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BLAKE - A THERMODYNAMICS CODE BASED ON
TIGER: USERS' GUIDE AND MANUAL

Eli Freedman

July 1982

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US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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third virial coefficient is computed for a hard-sphere model. Appropriate mixing rules are used for intermolecular force constants and for the virial coefficients.

Another valuable feature of the code is that it contains enthalpy data for 49 of the ingredients most often found in military propellants and for the 300 nitrocelluloses with percentages of nitration between 11.00 and 14.00.

This report is a complete guide to the local implementation and use of the code. It contains illustrative examples of its use, and its application to the AUTOCAP exercise, and a discussion of its experimental validation.

2
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TABLE OF CONTENTS

	Page
LIST OF TABLES	5
I. PREFACE.	7
A. Target	7
B. Notation and Usage	7
C. Applicability of This Report	7
II. INTRODUCTION	7
A. Some Background.	8
B. Comments on Gaseous Equations of State	11
C. Algebra of the Truncated Virial Equation	11
III. COMPUTATIONAL AND EXPERIMENTAL TESTS OF 'BLAKE'.	14
A. Computational Test	14
B. Experimental Test.	19
IV. APPLICATION OF 'BLAKE' TO THE AUTOCAP EXERCISE	20
V. SOURCES OF DATA.	32
A. Elements	32
B. Product Species.	32
C. Ingredients.	33
VI. IMPLEMENTING 'BLAKE'	36
A. Machine-Dependent Features	36
B. User-Dependent Aspects	39
VII. USING 'BLAKE'.	39
A. Job Control Cards and the First Two Runs	39
B. Comments on the Computation of Equilibrium by TIGER.	40
C. General Remarks on the Instruction Set	42
D. The Instruction Set.	43
E. Error Messages	57

TABLE OF CONTENTS (Continued)

	Page
VIII. THE OUTPUT FROM 'BLAKE'	64
IX. ACKNOWLEDGMENTS.	68
REFERENCES	69
APPENDIX A	71
APPENDIX B	75
APPENDIX C	99
DISTRIBUTION LIST.	125

LIST OF TABLES

Table	Page
1 Formulations for Code Intercomparison	15
2 Comparison of BLAKE with NASA/Lewis	16
3 Comparison Between ICT Code and BLAKE (Ideal Gas Case). .	18
4 Comparison of Results from the ICT Code and BLAKE (Real Gas Case)	22
5 BLAKE Computations on Crow-Grimshaw's Propellants	23
6 Vest's Experiments.	26
7 Relative Force of AUTOCAP Propellants	28
8 Parametric Sensitivities of AUTOCAP Lots.	29
9 Variability of Ingredients in AUTOCAP M-6	30
10 Names and Abbreviations of the Pre-Stored Ingredients in BLAKE	34

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I. PREFACE

A. Target

This report is designed for YOU, the user, and is so written.

B. Notation and Usage

The numeral '0' (zero) and the letter 'O' (oh) are easily confused. In this report, the character 'O' is always the letter when it appears with other letters, as in COM or ORD. If it appears with numbers, as in 3.04 or 1.0, it is a numeral. In a few places where misunderstanding may occur, the symbol 'Ø' is used for the letter 'oh'. (This is standard BRL usage.)

In this report, certain names appear inside single quote marks, as 'name2'. When this happens, you are to understand that it is the quantity denoted by the symbol 'name2' that is being referred to, not the characters themselves. (This is contrary to standard computer usage, but is adopted here in order to minimize the use of quote marks.)

In standard American English usage, punctuation marks go inside quote marks. In this report, however, the punctuation is placed outside the quote marks to decrease the likelihood of confusion.

C. Applicability of This Report

Since late 1978, BLAKE has printed a version designator on every output page. This report is specifically intended for use with version 205.0. Any change in the program, no matter how small, will be signalled by a change in version number.

In any case, the nature of the change or correction will be noted in comment cards placed in Subroutine VRSION. If necessary, changes to this manual will be noted there also.

II. INTRODUCTION

The BLAKE computer program is a general equilibrium thermodynamics program derived from an older version of TIGER. Although it is applicable to a wide range of chemical equilibrium calculations, it is specifically intended for computing the properties of gun propellants at chamber conditions.

A. Some Background

Among the first chemical equilibrium programs that did not assume the ideal gas equation were BKW and RUBY. They both employed the Becker-Kistiakowsky-Wilson equation of state that had been developed earlier at Los Alamos for the computation of p-V-T properties behind detonation waves in condensed explosives. RUBY apparently was difficult to use, requiring considerable user supervision and intervention. To improve this situation, the US Army Ordnance Corps' Ballistic Research Laboratories (now the Ballistic Research Laboratory of the US Army Armament Research and Development Command) contracted with the Stanford Research Institute (now Stanford Research International) to develop an entirely new code that would be much easier to use and that would permit the ready insertion of a variety of non-ideal equations of state for the gaseous and condensed states. The TIGER code was the result. Since then, managerial oversight of TIGER has resided in a group representing the Army, Navy, and Energy Departments. Under its guidance, the program has been significantly improved and its capabilities extended.

Originally TIGER incorporated only two gaseous equations of state, the ideal and the BKW, neither of which is applicable to gases at gun-chamber conditions. These are typically pressures up to 700 MPa and temperatures between 1500 and 3000 K, too dense for the ideal gas equation but not nearly dense enough for the BKW. A more appropriate equation for such conditions is the truncated virial equation,

$$pV = nRT [1 + (n/V)B(T) + (n/V)^2C(T)], \quad (1)$$

whose application to this problem was first described by Corner¹.

Corner showed how the constants B(T) and C(T), the second and third virial coefficients, could be computed once the intermolecular potential was known. The significance of this result is that it bypasses the need for measurements on the chamber gases, a complex mixture of some 10 to 40 molecules, free atoms, and radicals, at elevated temperatures and pressures.

A code embodying Corner's results was written over 22 years ago in the BRL by Leser². Results obtained with it were summarized in a comprehensive report by Baer and Bryson³ which is still a valuable reference work.

¹J. Corner, *"Theory of the Interior Ballistics of Guns,"* J. Wiley & Sons, NY & London (1950).

²T. Leser, *"High Speed Digital Calculations of the Composition and Thermodynamic Properties of Propellant Gases by the Brinkley Method,"* BRL R1023 (August 1957) (AD 156716)

³P. G. Baer and K. Bryson, *"Tables of Computed Thermodynamic Properties of Military Gun Propellants,"* BRL MR 1338 (March 1961). (AD 258644)

Leser's program was written in assembly language for ORDVAC. Some years later, Baer and Wortman produced a new version of the program in a high-level language called FORAST. The Baer-Wortman program is documented in an appendix to a report by Stansbury and Shearer⁴. This latter program became a veritable work-horse within the BRL, but it could not be exported because the explosive acceptance of FORTRAN negated the possibility of FORAST compilers being written elsewhere.

When the use of FORAST was proscribed, the TIGER⁵ code was already available. One of TIGER's many outstanding features is its modular design, which enables one to insert other gaseous equations of state by changing only one subroutine. Rather than translate Baer-Wortman, it was decided to take advantage of TIGER and thus gain the benefits of TIGER's other attractive features. The result was BLAKE.

From a common origin in 1964 TIGER and BLAKE have proceeded along separate paths; both programs have changed so much that their 1979 versions cannot use input cards prepared in 1964. The improvements in TIGER have always broadly emphasized the computation of detonation parameters, including improved convergence, two-phase systems, and partially-frozen expansions. Consequently it remains the code of choice for detonation computations for condensed explosives. BLAKE has continued to emphasize gun propellants; in its present form, its original capabilities for computing Chapman-Jouguet parameters and Hugoniot curves have been deleted.

B. Comments on Gaseous Equations of State

The truncated virial equation is nowadays primarily of theoretical significance only. Practicing chemical engineers have at their disposal many better equations (e.g., Benedict-Webb-Rubin, Beattie-Bridgman). These equations cannot be used for propellant-gas computations because there is no feasible way of finding the values of their many parameters; the Benedict-Webb-Rubin equation, for instance, has 8.

⁴L. Stansbury, Jr. and R. B. Shearer, "Tables of Computed Thermodynamic Properties of Selected Liquid Monopropellants," BRL R1579 (April 1972). (AD 521326L)

⁵a) W. E. Wiebenson, Jr., W. H. Zwisler, L. B. Seely, and S. R. Brinkley, Jr., "TIGER Computer Program Documentation (November 1968);

b) M. Cowperthwaite and W. H. Zwisler, "TIGER Computer Program Documentation," SRI Publication No. Z106 (January 1973).

The significance of Corner's work is that, although the truncated virial equation is far from the best, it is exceptionally useful. Corner used the Lennard-Jones 6,12 intermolecular potential function,⁶

$$\phi(r) = 4(\epsilon/kT)[(\sigma/r)^6 - (\sigma/r)^{12}] \quad (2)$$

where

- $\phi(r)$ = intermolecular potential;
- ϵ = depth of the attractive well;
- σ = distance at which the attraction vanishes; and
- r = distance between two molecules.
- h = Boltzmann constant, and
- T = absolute temperature

The exponent 6 is dictated by theory; the exponent 12 was chosen to give the best fit for second virial coefficients.

A drawback of the Lennard-Jones potential is that it is inherently incapable of representing the intermolecular potentials of either non-spherical or polar molecules, especially water. The Stockmayer potential⁷, which adds the term $-\mu^2 G/r^3$ (μ = dipole moment, and G = a function of the angles that specify the orientation of the dipole in space) to Eqn. (1), was developed to overcome this objection.

Unfortunately the situation is too complicated to be redeemed by a single extra term. While the Stockmayer potential does give improved estimates for $B(T)$, it does not improve the estimates of $C(T)$.

Numerically the contribution of the third coefficient is necessary for loading densities greater than about 0.2 g/cm^3 , but theory does not appear capable of giving adequate estimates for it. For this reason, BLAKE eschews the complications inherent in making extensive theoretical estimates of $C(T)$; instead, it follows an earlier recommendation of Hirschfelder's⁸ and computes the third virial coefficient with the assumption that the molecules are hard spheres with a radius equal to 0.81 times the Lennard-Jones radius σ .

⁶For a thorough discussion of gaseous equations of state and their relation to intermolecular potentials, see J.O. Hirschfelder, C.F. Curtiss, and R.B. Bird, "Molecular Theory of Fluids," John Wiley & Sons, New York (1954).

⁷See the discussion in ref. 6.

⁸See ref. 6, p. 157 and pp. 262-263.

This decision was made early during the development of BLAKE. In 1977 a coding error was discovered in this part of the code; in retrospect, it would have been better to have changed the model from hard spheres to square wells at that time, but....

Corner's approach applied strictly only to A-A and B-B interactions in a mixture of A and B; A-B interactions were ignored. Although it may be inconsistent with the neglect of sophisticated third-virial computations, the present BLAKE employs mixing rules for both the parameters of the intermolecular potential and of the virial coefficients. They are:

$$\epsilon_{ij} = [\sigma_i^3 \sigma_j^3]^{1/2} \sigma_{ij}^{-3} [\epsilon_i \epsilon_j]^{1/2}; \quad (3)$$

$$\sigma_{ij} = 0.5(\sigma_i + \sigma_j); \quad (4)$$

$$B(T) = \sum_i \sum_j x_i x_j B_{ij}; \text{ and} \quad (5)$$

$$C(T) = \sum_i x_i C_{iii}. \quad (6)$$

In these equations, x_i and x_j are the mole fractions of species i and j (which may be the same), B_{ij} is the virial coefficient for the mixture of gaseous species i and j (computed using the parameters ϵ_{ij} and σ_{ij} ; and $B(T)$ and $C(T)$ are the second and third virial coefficients of the total mixture.

Note that the mixing rule for the third virial coefficient is simply a linear weighted sum, with all interactions ignored. This is consistent with the use of the hard-sphere model.

C. Algebra of the Truncated Virial Equation

The insertion of a new gaseous equation of state into TIGER requires the evaluation of a number of expressions which are then programmed and put into Subroutine STATEG.

For reference purposes, these expressions are given here for the truncated virial equation. The exposition is not to be considered a derivation.

The truncated virial equation is

$$p = (RT/V) [1 + (B/V) + (C/V)^2] \quad (7)$$

for 1 mole of gas of volume V . Here R is the universal gas constant, and B and C are the second and third virial constants.

A completely general equation of state is

$$p = nRT\phi\rho/M_0 \quad (8)$$

If $\phi = 1$, this becomes the ideal gas equation of state; in general, ϕ is a measure of the deviation from ideality.

In the general case, B and C are functions of temperature, but here, C will be assumed independent of temperature.

The volume, V, is related to the reference mass, M_0 , and the density, ρ , by

$$\rho = M_0/V \quad (9)$$

The following quantities will also be needed:

x_i : mole fraction of i

n_i : moles of i

n : total moles = $\sum n_i$

then,

$$\begin{aligned} B &= \sum x_i x_j B_{ij} \\ &= \sum (n_i n_j / n^2) B_{ij} \end{aligned} \quad (10)$$

$$C = \sum (n_i / n)^3 C_i \quad (11)$$

$$\begin{aligned} P &= nRT\rho\phi/M_0 \\ &= (nRT\rho/M_0) [1 + (Bn\rho/M_0) + (n\rho/M_0)^2 C] \end{aligned} \quad (12)$$

The TIGER formalism requires the quantities $\partial P/\partial n_i$, Γ_i , $\partial \ln \phi/\partial \ln T$, $\partial \ln \phi/\partial \ln \rho$, $\partial \ln \phi/\partial n_i$, $\partial \Gamma_i/\partial \ln T$, $\partial \Gamma_i/\partial \ln \rho$, $\partial \Gamma_i/\partial n_j$, e , and ϵ_T .

Some of these have already been defined, the others are

$$\Gamma_i = \int_0^\rho [(M_0/RT\rho)(\partial \rho/\partial n_i) - 1] d\rho/\rho \quad (13)$$

$$\epsilon = \int_0^\rho (M_0/RT\rho) [\rho - (\partial \rho/\partial T)T] d\rho/\rho, \text{ and} \quad (14)$$

$$\epsilon'_T = \int_0^\rho (M_0 T/R\rho) (\partial^2 \rho/\partial T^2) d\rho/\rho \quad (15)$$

The origin and physical meanings of all of these quantities are in the TIGER documentation and will not be duplicated here.

When the truncated virial equation (with constant C) is substituted into these expressions, tedious algebra leads to the following equations:

$$p = (nRT\rho/M_o) + (\rho/M_o)^2 RT \sum_i n_i n_j B_{ij} + (\rho/M_o)^3 RT \sum_i n_i^3 C_i \quad (16)$$

$$r_i = (2\rho/M_o) \sum_j n_j B_{ij} + (5/2)(\rho/M_o)^2 n_i^2 C_i \quad (17)$$

$$\phi = 1 + (\rho/M_o n) \sum_i n_i n_j B_{ij} + n(\rho/M_o n)^2 \sum_i n_i^3 C_i \quad (18)$$

$$\partial \ln \phi / \partial \ln T = (\rho/\phi) \{ (1/M_o n) \sum_i n_i n_j B_{ij} + (2\rho/M_o^2 n) \sum_i n_i^3 C_i \} \quad (19)$$

$$\partial \ln \phi / \partial n_i = (\rho/M_o n \phi) \{ 2 \sum_j n_j B_{ij} - (1/n) \sum_i n_i n_j B_{ij} + (\rho/M_o) [3 n_i^2 - \{ (n_i^3/n) \} C_i] \} \quad (20)$$

$$\partial r_i / \partial \ln T = (2\rho T/M_o) \sum_j n_j \partial B_{ij} / \partial T \quad (21)$$

$$\partial r_i / \partial \ln P = r_i + (5/2)(\rho/M_o)^2 n_i^2 C_i \quad (22)$$

$$\partial r_i / \partial n_j = (\rho/M_o) \{ 2 B_{ij} + (3\rho/M_o) n_j^2 C_j \sigma_{ij} \} \quad (23)$$

(σ_{ij} is the Kronecker function, defined as

$$\sigma_{ij} = 0 \text{ if } i \neq j, \sigma_{ii} = 1.) \quad (24)$$

$$\varepsilon = -(\rho T/M_o) \sum_i n_i n_j \partial B_{ij} / \partial T \quad (25)$$

$$\varepsilon'_T = -(\rho/M_o) \sum_i n_i n_j \{ 2 T d B_{ij} / d T + (T^2/M_o) d^2 B_{ij} / d T^2 \} \quad (26)$$

I want to thank Arthur Cohen for checking the algebra (and finding an error), and Caledonia Henry for double-checking the algebra and checking the programming required to inject these equations into the code.

III. COMPUTATIONAL AND EXPERIMENTAL TESTS OF 'BLAKE'

A. Computational Test

The computational testing of BLAKE has two aspects. The first, which is readily accomplished, is verifying that the code produces the correct results for thermodynamic computations on ideal gases. One could do this by hand calculations but the ready availability of several well-validated codes makes this unnecessarily laborious. The NASA-Lewis code, CEC⁹, was taken to be the standard. Computations were run on it for five different propellant formulations. These five propellants were chosen not as representative, current, or typical, but mainly to ensure that the temperature range from 2250 to 3890 K was covered, and that at least one of them formed a condensed phase. Loading densities from 0.05 to 0.40 in intervals of 0.05 were used; some calculations at a loading density of 0.60 were also made. All calculations used the same enthalpies of formation as input.

A code developed by the Institut fuer Chemie der Treib- und Explosivstoffe¹⁰ was also run.

The results are described in another report¹¹, but it is very inaccessible so they will be repeated here.

The five compositions are shown in Table 1, and the results in Table 2. The concordance is excellent. Additional evidence for the quality of the agreement is found in the M15 calculations where BLAKE and CEC⁹ both predict the formation of liquid Al_2O_3 with mole fractions of 0.000124 and 0.00012, respectively.

The agreement between BLAKE and the ICT code is shown in Table 3. It is also very good, but not quite so perfect as between NASA-Lewis and BLAKE. The reason likely is in the thermodynamic data selected for the products.

⁹S. Gordon and B. J. McBride, "Computer Program for Computation of Complex Chemical Equilibrium Compositions....," NASA SP-273 (1971).

¹⁰F. Volk and R. Bathelt, "Application of the Virial Equation of State in Calculating Interior Ballistic Quantities," Propellants and Explosives 1, 7-14 (1976)

¹¹E. Freedman, "An Intercomparison of West German and US Propellant Thermodynamic Codes," in Agenda of Presentations at the 25-28 April 1978 Meeting of the FRG and US Personnel Associated with DEA 1060, p. IB-V-119 (April 1978).

TABLE 1. FORMULATIONS FOR CODE INTERCOMPARISON

<u>Ingredient Abbreviation</u>	<u>One</u>	<u>Two</u>	<u>Three</u>	<u>Four</u>	<u>Five</u>
NC	83.173	19.940	45.954	58.330	79.600
(% N in NC)	(12.60)	(13.15)	(13.15)	(13.25)	(13.15)
NG	--	18.943	21.478	40.400	9.950
NQ	--	54.536	30.669	--	--
DNT	9.843	--	--	--	--
DBP	4.429	--	--	--	8.955
KCRY	--	0.299	--	--	--
DPA	0.984	--	--	--	0.295
EC	--	5.982	1.50	0.760	--
ETOH	0.98	0.300	0.30	0.510	0.500
H ₂ O	0.59	0.0	0.0	0.0	0.0
C	--	--	0.100	--	--

All ingredients are assumed to be distributed homogeneously for the purposes of computation.

TABLE 2. COMPARISON OF BLAKE WITH NASA/LEWIS

I D E A L G A S						
LOADING DENSITY (g/cm ³)	BLAKE		NASA-Lewis		% Differences	
	T (K)	P (MPa)	T (K)	P (MPa)	T	P
			ONE			
0.2	2266.	173.7	2265.	173.6	0.04	0.07
0.4	2285.	347.9	--	--	--	--
0.5	2295.	435.3	2295.	434.8	0.0	0.10
0.6	2306.	522.8	--	--	--	--
			TWO			
0.2	2559.	197.5	2558.	197.4	0.04	0.06
0.4	2563.	394.8	--	--	--	--
0.5	2565.	493.4	2565.	493.0	0.0	0.08
0.6	2567.	591.9	--	--	--	--
			THREE			
0.2	3221.	221.8	3220.	221.7	0.03	0.07
0.4	3230.	444.5	--	--	--	--
0.5	3232.	555.8	3230.	555.3	0.06	0.10
0.6	3234.	667.2	--	--	--	--
			FOUR			
0.2	3815.	235.6	3813.	235.5	0.05	0.06
0.4	3865.	475.7	--	--	--	--
0.5	3880.	596.2	3877.	595.6	0.08	0.10
0.6	3891.	716.8	--	--	--	--
			FIVE			
0.2	2602.	192.6	2600.	192.4	0.08	0.10
0.4	2604.	288.8	--	--	--	--
0.5	2608.	481.3	2606.	480.6	0.08	0.14
0.6	2610.	769.8	--	--	--	--

Although they employ different fittings for them, BLAKE and CEC71 both use virtually the same numbers from the JANNAF Tables¹²; it is not clear which data were used in the ICT calculations.

Also, I have occasionally made spot checks of BLAKE runs against the new TIGER code; here, too, the results are in excellent agreement.

It is concluded that BLAKE gives consistently accurate thermodynamic results for the ideal gas case.

The non-ideal gas case is more difficult to test because there is no generally-accepted standard code that can be used as a standard. The best that one can do is to compare one code against the other. The results are in Table 4. The agreement is surprisingly good, especially when one considers the difference in approach between them. The maximum discrepancy in pressure does not exceed 3.5%, and that occurs at a loading density of 0.6 g/cm³, a figure that approaches the density of some liquids! The column labeled ϕ gives the ratio of the computed pressure to the ideal-gas pressure for the same conditions. At a loading density of 0.6, ϕ is 2.1; that is, the correction factor for the ideal pressure is 110%.

Klein et al.¹³ have proposed a new equation of state specifically for ballistics. Their treatment includes a term for the interaction between water and carbon dioxide, a specific interaction that is ignored in BLAKE. It will be interesting to see the magnitude of the change that this equation will produce in ballistic calculations; unfortunately, inserting the equation into BLAKE has turned out to be far from a routine matter¹⁴.

¹²D. R. Stull and H. Prophet, Eds., "JANAF Thermochemical Tables," 2nd ed., NSRDS-NBS 37 (June, 1971); also looseleaf revisions and additions from the Thermal Research Laboratory, The Dow Chemical Company, Midland, MI (M. Chase, Director).

¹³E. G. Powell, G. Wilmot, L. Haar, and M. Klein, "Equations of State and Thermodynamic Data for Interior Ballistics Calculations," in H. Krier and M. Summerfield, *Interior Ballistics of Guns, Progress in Astronautics and Aeronautics*, vol. 66, AIAA, New York (1979).

¹⁴M. Klein, (National Bureau of Standards), private communication to E. Freedman; February 1980.

TABLE 3.
COMPARISON BETWEEN ICT CODE & BLAKE
IDEAL GAS CASE

Name	Temperature (K)		Pressure (MPa)		Impetus (J/g)	
	ICT	BLAKE	ICT	BLAKE	ICT	BLAKE
<u>One</u>						
0.2	2265	2270	173.6	174.0	867.8	870.0
0.4	2284	2290	347.6	348.5	869.0	871.3
0.6	2306	2311	522.2	523.7	870.3	872.8
<u>Two</u>						
0.2	2558	2560	197.4	197.5	987.2	987.6
0.4	2563	2564	394.6	394.9	986.6	987.1
0.6	2568	2568	591.6	592.0	986.0	986.5
<u>Three</u>						
0.2	3220	3223	221.8	222.0	1109.	1110.
0.4	3229	3232	444.2	444.7	1111.	1112.
0.6	3233	3236	666.7	667.6	1111.	1113.
<u>Four</u>						
0.2	3816	3814	235.7	235.7	1178	1178.
0.4	3865	3865	475.5	475.7	1189	1189.
0.6	3890	3891	716.4	716.9	1194	1195.
<u>Five</u>						
0.2	2600	2609	192.4	193.1	962.0	965.5
0.4	2604	2613	384.6	386.1	961.6	965.3
0.6	2608	2617	576.7	579.0	961.2	965.1

Pending this development, one can take some comfort from the agreement between BLAKE and the ICT code; it would be indeed surprising if both codes were wildly wrong. In my opinion, the agreement mostly shows the profundity of Hirschfelder's insight⁸ of years ago: the computations are insensitive to the differences in models in the range of temperatures that is ballistically interesting.

B. Experimental Test

The over-all conclusion must be that BLAKE results are worthy of credence, but the desirability of experimental confirmation is not thereby lessened. The principal difficulty with such a test is the determination of the true equilibrium pressure, the maximum pressure that would be reached in a closed bomb if there were no heat loss. This heat loss causes a drop in the measured pressure. In 1931 Crow and Grimshaw¹⁵ published an important paper which reported such an attempt. Their pioneering work necessarily had to use a simplified model of the heat loss mechanism in order to achieve results. A decade later Kent and Vinti¹⁶ commented that the thermodynamic calculation of the equilibrium temperature was theoretically more sound; they used this temperature in a new model of heat loss and were thus able to compute a corrected pressure. All later workers have followed this lead.

In 1953 Vest¹⁷ reasoned that heat loss in a closed bomb should decrease with surface-to-volume ratio. He made measurements in bombs containing added metal pieces and then computed a corrected pressure by extrapolation of the measured pressures back to a surface-to-volume ratio of zero. Vest's compositions are listed in Appendix A.

Table 5 presents the final pressures computed by Crow and Grimshaw from their measurements and the pressures computed with BLAKE for their compositions. These compositions are also listed in Appendix A. These calculations were made without considering the contribution of the acetylene/air igniter that was used, which would add 0.2 MPa or less to the results.

¹⁵A. D. Crow and W. E. Grimshaw, "The Equation of State of Propellant Gases," *Phil. Trans. Roy. Soc. A* 230, 30 (1931).

¹⁶R. H. Kent and J. P. Vinti, "Cooling Corrections for Closed Chamber Firings," BRL R 281 (September, 1942). (AD 492852)

¹⁷D. Vest, "On the Transfer of Heat in High-Pressure Combustion Chambers," unpublished M. S. Thesis, The Johns Hopkins University, Baltimore, Maryland (1953).

The agreement at loading densities above 0.07 g/cm^3 is as good as one could ask. Crow and Grimshaw themselves noted that their treatment of the heat loss was questionable at the lower densities. Also, Kent and Vinti's correction is much larger in that region; their correction is much smaller at the higher densities, and their final pressures are only slightly lower than Crow and Grimshaw's.

Vest's results are shown in Table 6; they are much less extensive than Crow and Grimshaw's. The table also gives the BLAKE results. The agreement is good only at the loading density of 0.15. The poorer agreement at the two lower densities may indicate a failure of Vest's model.

The present state of the art in closed-bomb experimentation makes it easier to conduct experiments at even higher pressures than those used by Crow and Grimshaw. Such experiments should certainly be undertaken; also, the Crow-Grimshaw treatment at higher loading densities deserves another look.

IV. APPLICATION OF 'BLAKE' TO THE AUTOCAP EXERCISE

An excellent example of the utility of BLAKE is given by its application to the AUTOCAP exercise. One of the purposes of this exercise was to determine the effects of variation in composition on the performance of propellants. To this end, many lots of M-6 propellant were made with deliberate changes from the accepted specification. Among numerous other properties, the impetuses of these lots were determined; also, the impetus of a reference lot of M-6 was measured. The ratio of the measured impetus of a lot to the measured impetus of a standard or reference lot is called the relative force (RF).

Table 7 gives the measured and computed impetuses and the corresponding relative forces. The average deviation of the 9 lots is 0.6 with a standard deviation of 0.7. This means that the mean deviation is not significantly different from zero. This calculation has not been attempted with another code; it would be interesting to do so.

Another interesting and useful application of BLAKE is the computation of the effect on the impetus of small changes in composition or of ingredient properties. This quantity can be called the parametric sensitivity to distinguish it from other sensitivities (e.g., ignition sensitivity) to which it is unrelated.

Mathematically this quantity is $\partial P / \partial Q$, which can be approximated by $\Delta P / \Delta Q$. Here, P is a thermodynamic property such as impetus, maximum pressure, temperature, or ratio of heat capacities, and Q is the amount of an ingredient or a property of an ingredient. Thus one can calculate

the rate of change of maximum pressure with respect to the amount of dinitrotoluene, or the rate of change of the ratio of heat capacities with respect to the heat of formation of nitrocellulose, etc.

The partial derivative notation implies that all other constituents are kept constant. This cannot actually be so, since it is only percentage composition that counts. Hence the partial derivative must be computed with the additional constraint that the sum of all of the constituents is a constant. In computing $\Delta P/\Delta Q$, the effect of the change in Q on the other constituents was in every case distributed over these other materials in proportion to their percentage in the original formulation.

Since impetus or maximum pressure cannot be readily expressed as a function of composition in closed form, the derivative $\partial P/\partial Q$ must be approximated by a discrete formula. The simplest correct one is

$$\partial P/\partial Q \approx (1/2h) [P(Q + h) - P(Q - h)], \quad (27)$$

where h is a small increment in Q. This formula approximates the derivative at the given value of Q. In order to decrease the amount of computation, the simpler but less correct formula:

$$\partial P/\partial Q \approx (1/h) [P(Q + h) - P(Q)] \quad (28)$$

was used. The increment h was generally chosen to be a convenient size, generally 10% of the base value of Q.

The results of the computations are given in Table 8. The significance of these numbers is best seen by looking at the last columns of this Table. It gives the approximate percentage change in impetus, F, or γ that would be brought about by a one percent change in that ingredient. In the case of the nitrogen content, the number is the percentage change in F for a change of 0.01 in the percentage of N.

Increases in either the amount of NC or the fraction of nitrogen in the NC cause an increase in the impetus; addition of all the other components causes a decrease. The reason for this is clear: increasing either NC or the fraction of nitrogen increases the energy of the propellant, hence the positive sign. Addition of the other substances caused an effective decrease in the amount of NC, and hence decreases the impetus. Note that the magnitudes of almost all of these quantities are not very different from each other. This also is a result of the fact that the principal effect of adding substance Q is to decrease the amount of NC (unless Q is itself NC).

Only the derivative for DNT is markedly different. This is because DNT is also an energetic substance, unlike the other additives. Hence,

TABLE 4
COMPARISON OF RESULTS FROM THE ICT CODE AND BLAKE
REAL GAS CASE

Compo- sition	T (K)		P (MPa)		Impetus (J/g)		Covolume (cm ³ /g)		ϕ	
	ICT	BLAKE	ICT	BLAKE	ICT	BLAKE	ICT	BLAKE	ICT	BLAKE
One										
0.2	2288	2284	227.5	225.0	873.0	872.1	1.163	1.123	1.3	1.3
0.4	2348	2347	600.9	585.6	874.7	877.3	1.044	1.002	1.7	1.7
0.6	2402	2427	1154.	1133.0	868.3	881.3	0.914	0.889	2.1	2.1
Two										
0.2	2573	2565	254.9	254.9	991.6	988.5	1.110	1.122	1.3	1.3
0.4	2590	2583	664.4	659.2	988.5	987.4	1.012	1.002	1.7	1.7
0.6	2613	2617	1267.	1264	978.0	984.7	0.895	0.887	2.1	2.1
Three										
0.2	3238	3233	279.1	280.0	1114.	1112	1.006	1.027	1.3	1.3
0.4	3251	3248	713.7	710.6	1116.	1116	0.935	.930	1.6	1.6
0.6	3247	3257	1355.	1341	1112.	1115	0.846	0.834	2.0	2.0
Four										
0.2	3852	3850	294.1	293.3	1188	1186	0.962	.956	1.2	1.2
0.4	3920	3922	750.9	737.6	1203	1202	0.898	0.870	1.5	1.5
0.6	3948	3963	1424	1377	1208	1211	0.819	.787	1.9	1.9
Five										
0.2	2612	2615	248.4	247.0	965.4	966.9	1.113	1.086	1.3	1.3
0.4	2624	2634	648.1	634.3	962.4	967.4	1.015	.975	1.6	1.6
0.6	2641	2671	1240.	1210	952.5	967.0	0.898	0.867	2.1	2.1

TABLE 5
BLAKE COMPUTATIONS ON CROW-GRIMSHAW'S PROPELLANTS
(All pressures are in MPa)

Loading density (g/cm ³)	N(1)			N(2)			N(3)		
	P(B)	P(O)	% diff	P(B)	P(O)	% diff	P(B)	P(O)	% diff
.0263	26.9	31.6	+17.	26.9	28.6	+6.6	26.0	27.9	7.0
.042	43.8	48.2	+10.	43.7	46.2	5.6	42.4	45.6	7.7
.0585	62.2	67.1	+8.	62.1	64.1	3.3	60.2	67.8	4.3
.0755	81.9	85.1	+4.0	81.8	84.6	3.5	79.2	79.6	0.5
.1066	119.8	122.9	+2.6	119.8	121.6	1.5	116.2	116.2	0.1
.1344	156.1	160.7	+3.0	156.2	155.7	-0.3	151.5	153.1	1.1
.1546	183.8	188	+2.3	184.1	184.2	0.1	178.6	177.1	-0.8
1819	223.3	226.9	+1.7	223.8	225.0	0.6	217.2	215.7	-0.7
2049	258.4	264.9	+2.5	259.1	258.8	-0.1	251.7	251.2	-0.2
.2211	284.2	286.7	+0.9	285.1	283.6	-0.5	277.0	277.0	0.0
.2479	328.6	330.6	+0.6	330.1	328.6	-0.4	321.0	320.4	-0.2

TABLE 5 (Continued)

BLAKE COMPUTATIONS ON CROW-GRIMSHAW'S PROPELLANTS

(All pressures are in MPa)

Loading density (g/cm ³)	C(1)		Δ	C(2)			%	C(3)		
	P(B)	P(O)		P(B)	P(O)	P(B)		P(B)	P(O)	%
.0263	30.4	34.2	12.8	30.4	36.0	NA	18.4	29.8	29.8	--
.0420	49.8	54.5	9.7	49.8	50.5	49.8	1.5	50.5	50.5	1.4
.0585	71.0	75.0	5.8	71.0	71.6	71.0	0.9	71.6	71.6	.9
.0755	93.7	95.9	2.3	93.7	93.4	93.6	-0.3	93.4	93.4	-1.3
.1066	137.6	139.2	1.3	137.6	136.7	137.3	-0.5	136.8	136.8	-0.4
.1344	179.5	179.8	0.3	179.4	176.5	179.0	-1.4	176.5	176.5	-1.4
.1546	211.5	210.6	-0.2	211.4	209.5	210.9	-0.7	208.8	208.8	-0.7
.1819	257.0	256.6	0.1	256.8	252.5	256.2	-1.5	253.1	253.1	-1.4
.2049	297.4	296.5	-0.1	297.1	293.5	296.4	-1.0	293.5	293.5	-0.1
.2211	327.0	325.8	-0.1	326.7	325.5	325.9	-0.8	323.9	323.9	-0.7
.2479	378.2	373.1	-1.1	377.9	374.3	377.0	-0.7	374.3	374.3	-0.7

TABLE 5 (Continued)

BLAKE COMPUTATIONS ON CROW-GRIMSHAW'S PROPELLANTS
(All pressures are in MPa)

Loading density (g/cm ³)	B(1)			B(2)			B(3)		
	P(B)	P(O)	%	P(B)	P(O)	%	P(B)	P(O)	%
0.0263	30.5	30.1	-1.4	30.5	36.0	17.9	30.5	31.9	4.4
0.042	50.2	52.3	4.2	50.2	55.1	9.9	50.2	52.6	4.8
0.058	71.7	74.0	3.5	71.7	77.1	7.6	71.7	77.1	7.5
0.0755	94.7	95.7	1.2	94.7	99.2	4.8	94.8	99.2	4.7
0.1066	139.4	139.0	-0.1	139.4	141.5	1.5	139.4	143.2	2.7
0.1344	182.0	184.3	1.6	182.0	183.0	0.8	182.0	183.2	0.7
0.1546	214.6	212.3	-0.7	214.6	216.0	0.7	214.6	215.6	0.5
0.1819	260.8	259.7	-0.1	260.8	260.6	-0.1	260.8	262.3	0.6
0.2049	302.0	301.1	0.1	301.9	300.5	-0.5	302.0	302.5	0.2
0.2211	332.1	332.2	0.4	332.0	331.8	-0.1	332.1	330.7	-0.4

TABLE 6
VEST'S EXPERIMENTS

Composition No. 1	P (MPa)	
	<u>Vest</u>	<u>BLAKE</u>
$\rho_L = 0.05$	43.7	48.9
0.10	96.8	104.2
0.15	159.4	166.7
Composition No. 2		
$\rho_L = 0.05$	54.2	57.7
.10	117.9	122.7
.15	193.2	195.0

while adding it decreases the percentage of NC, the net decrease in potential energy content is less because of the contribution that DNT makes.

Knowing the parametric sensitivities is not sufficient. We also need to know how closely the level of a particular ingredient can be controlled. A measure of this control is the standard deviation of each ingredient in successive lots. Table 9 gives such data¹⁸.

Together the numbers in Tables 8 and 9 can give an estimate of the variance of the muzzle velocity. We consider an "ideal" gun, one that has no energy loss due to heat conduction, engraving forces, etc., and one in which the propellant is completely burnt at shot start. For such a gun, the muzzle velocity, V , is

$$V^2 = (2cF/W(\gamma - 1))(1 - r^{\gamma-1}) \quad (29)$$

where r is the ratio of the volume of the chamber to the volume of the gun, c/w the ratio of charge weight to projectile weight, and F is the impetus. Variations in the components, Q_i , cause variations in F and γ , which in turn cause variations in V ; that is,

$$V = V[F(Q_i), \gamma(Q_i)], \quad (30)$$

where Q_i stands for the amounts of each of the components. Let V° be the average values of V . Then the effect of deviations from the averages of the Q_i can be expressed by a Taylor series:

$$V = V^\circ + \sum \left(\frac{\partial F}{\partial F} \frac{\partial F}{\partial Q_i} + \frac{\partial V}{\partial \gamma} \frac{\partial \gamma}{\partial Q_i} \right) (Q_i - Q_i^\circ) \quad (31)$$

The variance of V is defined by the expectation of the quantity $(V - V^\circ)^2$,

$$s_V^2 = \epsilon(V - V^\circ)^2 \quad (32)$$

This quantity will now be calculated.

¹⁸I. W. May, (Ballistic Research Laboratory), private communication to E. Freedman (1973).

TABLE 7
RELATIVE FORCE OF AUTOCAP PROPELLANTS

Lot	RF Measured	RF Computed	Deviation
A	100.98	100.25	-0.73
B	102.03	100.34	-1.69
C	100.72	99.72	-1.00
D	102.05	101.01	-1.04
E	99.78	99.40	-0.38
F	101.23	101.98	0.75
G	95.26	94.43	-0.83
H	95.08	94.80	-0.28
67994	100.54	99.29	-1.25
65306*	100.00	100.00	---

* Reference Lot

Mean deviation = -0.6
Standard deviation of mean = 0.7

TABLE 8

PARAMETRIC SENSITIVITIES OF AUTOCAP LOTS

<u>Variable</u>	$\frac{\partial F}{\partial Q}$	$\frac{\partial \gamma}{\partial Q}$	$\frac{1}{F} \frac{\partial F}{\partial Q}$	$\frac{1}{\gamma-1} \frac{\partial \gamma}{\partial Q}$
NC	3960	-0.0012	+0.013	-0.0047
DBP	-6150	~0	-0.020	~0
DPA	-6970	~0	-0.022	~0
K ₂ SO ₄	-6380	~0	-0.021	~0
H ₂ O	-4400	~0	-0.014	~0
ETOH	-5470	~0	-0.018	~0
DNT	-1220	+0.0018	-0.0039	+0.0071
% N in NC	+8100	~0	+0.026	~0

TABLE 9
VARIABILITY OF INGREDIENTS
IN AUTOCAP M-6

<u>Abbreviation</u>	<u>Substance</u>	<u>Average</u>	<u>Sigma</u>
% N	Percent N	13.146	0.0114
NC	Nitrocellulose	84.654	0.4936
DNT	Dinitrotoluene	10.137	0.4930
DBP	Dibutyl Phthalate	5.208	0.1478
DPA	Diphenylamine	1.009	0.0644
K ₂ SO ₄	Potassium Sulfate	1.086	0.1161
H ₂ O	Water	0.553	0.0931
ETOH	Alcohol	0.365	2.2466

$$s_V^2 = \sum_i^n \left[\frac{\partial V}{\partial F} \frac{\partial F}{\partial Q_i} + \frac{\partial V}{\partial \gamma} \frac{\partial \gamma}{\partial Q_i} \right]^2 \varepsilon(Q_i - Q_i^\circ)^2 + 2 \sum_{i>j}^n \left[\frac{\partial V}{\partial F} \frac{\partial F}{\partial Q_i} + \frac{\partial V}{\partial \gamma} \frac{\partial \gamma}{\partial Q_i} \frac{\partial V}{\partial F} \frac{\partial F}{\partial Q_j} + \frac{\partial V}{\partial \gamma} \frac{\partial \gamma}{\partial Q_i} \frac{\partial V}{\partial \gamma} \frac{\partial \gamma}{\partial Q_j} \right] \varepsilon(Q_i - Q_i^\circ)(Q_j - Q_j^\circ) \quad (33)$$

The quantity $\varepsilon(Q_i - Q_i^\circ)^2$ is the variance of Q_i , denoted $s^2(Q_i)$. The quantity $\varepsilon(Q_i - Q_i^\circ)(Q_j - Q_j^\circ)$ is the covariance of Q_i and Q_j , denoted by $\text{cov}(Q_i, Q_j)$.

The amounts of the several ingredients are subject to random variations; hence $s^2(Q_i) \neq 0$. But there is no special reason to believe that there is any relation between Q_i and Q_j ; it is just as likely that one of them will decrease while the other increases as it is that both will change in the same direction. Hence it is a reasonable assumption to set $\text{cov}(Q_i, Q_j) = 0$.

Differentiation gives

$$\partial V / \partial F = k f_1 / [2V(\gamma - 1)], \text{ and} \quad (34)$$

$$\partial V / \partial \gamma = -k F f_2 / 2V(\gamma - 1)^2, \quad (35)$$

$$\text{where} \quad f_1 = 1 - r^{\gamma-1}, \quad (36)$$

$$f_2 = f_1 + (\gamma - 1) (\ln r) r^{\gamma-1}, \quad (37)$$

$$\text{and} \quad k = (2gc/W)^{1/2} \quad (38)$$

There results after some algebra,

$$s_V^2 = (V/2f_1)^2 \left[f_1^2 \left(\frac{1}{F} \frac{\partial F}{\partial Q_i} \right)^2 + f_2^2 \left(\frac{1}{\gamma-1} \frac{\partial \gamma}{\partial Q_i} \right)^2 \right] s^2(Q_i) \quad (39)$$

A numerical example is enlightening. Choose

$$c = 15 \text{ kg},$$

$$W = 45 \text{ kg},$$

$$r = 0.2, \gamma = 1.253, \text{ and}$$

$$F = 10^6 \text{ J/kg}.$$

Then $V = 940$ m/s, and $s_V = 19$ m/s, or about 2%. This is a significant variation. Examination of the numbers that go into s_V shows that by far the major contributor in this case is the variability in the alcohol.

This result may appear paradoxical since the alcohol contributes virtually nothing to the impetus. As Sherlock Holmes might have said, that is just the point. The alcohol contributes nothing; an increase in its amount must come at the expense of the nitrocellulose, which does contribute a great deal. If the variability of the alcohol had been only 0.5 (the same as NC), the resultant s_V would have been 4 m/s, or about 0.4%, a tolerable amount.

V. SOURCES OF DATA

BLAKE is presently dimensioned to permit the simultaneous consideration of 29 gases and 10 condensed phases (liquids or solids or both) at one time; these species may contain up to 40 elements. In practice certain constraints (discussed in Sec. VII) must be considered.

A. Elements

BLAKE presently considers 16 elements: C, H, N, O, B, Al, F, Na, Ti, He, Ar, Ba, K, S, Cl, and Pb. Users may add another 24 without having to redimension any variables.

B. Product Species

Thermochemical data for 120 product compounds (98 gases and 22 condensed species) are included in the library furnished with BLAKE. The data for these compounds are taken without exception from the JANAF Tables¹². They are stored in the form of the coefficients of a linear combination of functions of $T/1000$ (T = absolute temperature); these coefficients were determined by a least-squares fitting and reproduce the data over the range 400 K - 5000 K. (See also Sec. VII C 1.)

The Lennard-Jones parameters were taken from the compilation of Reid and Sherwood¹⁹. In the many cases when no data are available, the program automatically substitutes $\epsilon = 300$ K and $\sigma = 3.5 \times 10^{-10}$ meter. The user can change these default values permanently at compile time by changing them in Subroutine LJPAR; or temporarily at run time by using the instruction LJP (Sec. VII C 2).

¹⁹Reid, R. C. and Sherwood, T.K., "The Properties of Gases and Liquids," 2nd ed., McGraw-Hill, New York (1966).

C. Ingredients

BLAKE contains enthalpies of formation for 349 different species in a DATA statement. Of these, 300 are nitrocelluloses with percentages of nitration varying from 11.00 to 14.00. These data are based on a re-working of those published by Jessup and Prosen²⁰ (including the correction of an obvious misprint). A least squares fitting of these data gives

$$\Delta h = -1406.22 + 6231.86 f, \quad (40)$$

where

Δh = enthalpy of formation (cal/g),

and

f = weight-fraction of nitrogen in the nitrocellulose.

Nitrocellulose with 100 f weight-percent nitrogen has the empirical formula $C_6H_{10-x}O_{5+2x}N_x$, where x is the number of nitrogen atoms in a monomeric unit, given by

$$x = 162.1430 f / (14.0067 - 44.9975 f) \quad (41)$$

The molecular weight corresponding to this empirical formula is

$$MW = 44.9975 + 162.1430f \quad (42)$$

The combination of these formulas with Jessup and Prosen's data gives the enthalpies of formation of all nitrocelluloses as a function of f .

The other 50 compounds are 49 of the most common ingredients used in the formulation of solid and liquid propellants. (One compound appears twice.) The names of these compounds and the abbreviations or acronyms adopted for them are listed in Table 10.

As much as possible, the acronyms or abbreviations were chosen to agree with customary and traditional usage. Ethanol appears twice, one as ALC for those who prefer the common abbreviation, and once as ETOH for those who appreciate the subtleties of organic nomenclature.

²⁰R. S. Jessup and E. J. Prosen, "Heats of Combustion and Formation of Cellulose and Nitrocellulose (Cellulose Nitrate)," J. Res. National Bureau of Stds. 44, 387-393 (1950).

TABLE 10

<u>Chemical Name</u>	<u>Abbreviation</u>
Acetone (dimethyl ketone)	ACETON
Alcohol (ethanol)	ALC
Amyl phthalate	AMYLPH
Akardite 2	AKAR2
Ammonium nitrate	AN
Barium oxide	BAO
Barium nitrate	BANITR
Basic lead oxide	PB2CO4
Carbon (graphite)	C
Cellulose diacetate	CEDAC
Cellulose nitrate -- see nitrocellulose	---
Cellulose triacetate	CETAC
Cryolite (sodium aluminum fluoride)	CRY
Cyclotetramethylene tetranitramine (octogen)	HMX
Cyclo-1,3,5-trimethylene-2,4,6-trinitramine (hexogen)	RDX
Decalin	DECA
Dibutyl phthalate	DBP
Diethyleneglycol dinitrate	DEGDN
2,2'-dinitrodiphenylamine	NNDP
Dinitrotoluene	DNT
Diphenylamine	DPA
Ethanol	ETOH
Ethanolamine nitrate	EOAN
Ether	ETHER
Ethyl centralite	EC
Ethylenediamine dinitrate	EDDN
Ethylene glycol	EGLY
Ethyl ether	ETHER
Glycerin	GLY
Graphite	C
H ₂ O (water)	H ₂ O
Hexogen	RDX
HMX	HMX
Hydrazine	N ₂ H ₄
Hydrazine nitrate	HN
Hydroxylammonium nitrate	HAN

<u>Chemical Name</u>	<u>Abbreviation</u>
Isopropylammonium nitrate	IPAN
Lead oxide (see also basic lead oxide)	PBO
Metriol	METRIO
Methyl centralite	MC
Nitrocellulose with vw.xy percent nitrogen	NCvwxy
2-nitrodiphenylamine	NDPA
Nitric acid	HNO3
Nitrogen	N2
Nitroglycerin	NG
Nitroguanidine	NQ
Octogen	HMX
Oxygen	O2
Pentaerythritol pentanitrate	PETN
Potassium nitrate	KN
Potassium sulfate	KS
Potassium tetrafluoroborate	K2F4
RDX	RDX
Sodium aluminum fluoride	CRY
Triacetin	TRIAC
Triaminotrinitrobenzene	TATB
Triethyleneglycol dinitrate	TEGDN
Trimethylammonium nitrate	TMAN
Unsymmetrical dimethyl hydrazine	UDMH
Water	H2O

The formulas and enthalpies of formation of these ingredients are listed in Appendix B. Wherever possible they were taken from the authoritative compilation of Cox and Pilcher²¹. Data for the inorganic compounds were taken either from the NBS compilation²² or from Lange's Handbook²³.

VI. IMPLEMENTING 'BLAKE'

A. Machine-Dependent Features

BLAKE is written almost exclusively in the extended set of American National Standard FORTRAN. There are six functions and one feature in it, however, that are system- or computer-dependent. These functions (CLOCKS, SECOND, DAY, ENCODE, DECODE, AND EOF) are used only in convenience features and can be readily omitted. The machine-dependent feature, word length, may cause a little more work.

1. Clock.

It is desirable but not essential that the program be capable of obtaining the current time from the system clock. As furnished, the program contains Subroutine CLOCKS(T). This subroutine returns the time in seconds from the previous midnight. BLAKE obtains this time from a system function named SECOND(T).

2. Date.

It is desirable but not essential that the program be capable of obtaining the current date from the system clock or calendar. As furnished, the program contains Subroutine DAY(IDAY). IDAY is an array of 20 alphanumeric characters that is later printed using a format of 20A1. BLAKE inserts the current date in the first 12 places, and blanks in the other 8. It does this using the machine-dependent functions ENCODE and DECODE. If you want this feature, you will have to make appropriate implementations of these functions.

²¹J. D. Cox and G. Pilcher, *"Thermochemistry of Organic and Organometallic Compounds,"* Academic Press, London (1970).

²²D. D. Wagman, et al., *"Selected Values of Chemical Thermodynamic Properties,"* NBS Technical Note 270-3, Washington, DC (1968).

²³J. A. Dean, ed., *"Lange's Handbook of Chemistry,"* 12th ed., McGraw-Hill, New York (1979).

3. EOF.

It is convenient but not necessary to check for the occurrence of an end-of-file mark in the input. BLAKE does this in Subroutine CARDRD after each READ instruction by use of the CDC function, EOF(LI), where LI is the logical unit number of the input device. You will probably have to change it for your particular computer.

The standard FORTRAN-77 statement

```
READ (unit, format, END=435)
```

is already in the program as a comment card. If your computer will recognize it, by all means use it.

4. Word Length.

TIGER, and hence BLAKE, proceed by interpreting a series of instructions. The detailed form of these instructions is given in Section VI; here it is only necessary to note that each separate field in an instruction is converted by the program (in Subroutine CARDRD) to a real number containing from 2 to 12 digits (2 digits per character). For example, the symbols

P, H20, 17E-3, and K2S04\$

become

30., 220229., 0107191303., and 250233290447.,

respectively. Some of these numbers are used as such; others, such as 220229 ('H20') are eventually converted back to their original alphanumeric form for printing. The conversion routine, Subroutine CONVRT, starts by converting the real number into integer form. Depending on the number of characters permitted, the routine may have to handle from 6 to 12 digits without the loss of even the least significant digit.

CDC computers can handle 12 digits without any loss, so BLAKE is set to accept 6 characters in Subroutine CARDRD. Most other computers cannot handle more than 8 digits (4 characters) and hence require changes in CARDRD.

The change is simple. Line 100 currently reads

```
IF (IFLAG - 6) 270, 280, 290
```

All that is needed is to change the '6' to a '4'. If your computer can only handle 6 or 7 digits, the '6' becomes a '3'.

Also, two changes are required in Subroutine LIBRAY. First, the line immediately after statement 1010 which now reads

```
IF (STR(J,2) - 3400000000.) 1020, 1020, 1060
```

must be changed to

```
IF (STR(J,2) - 30000000.) 1060, 1060, 1020
```

Secondly, the line immediately after statement 1120

```
IF (STC(J,2) - 3400000000.) 1140, 1140, 1130
```

must be changed to

```
IF (STC(J,2) - 30000000.) 1130, 1130, 1140
```

Two changes are needed in Subroutine BLAKEM. Statement 390 contains the number

```
2318201526. ;
```

it must be changed to

```
231820.
```

Statement 420 contains the number

```
362332231526. ;
```

it must be changed to

```
362332.
```

Finally, changes will be needed in the library itself.

1. The words SOLID, LIQUID, AND CONDENSE must be changed to SOLI, LIQU, and COND, respectively.

2. Many of the constituents in the library have six-character names; these must all be changed to four characters each. Be careful when making the changes to note two things:

a. All names must be unique; it is regrettably easy to introduce duplicates when shortening the existing names.

b. If possible, make the changes with a computer editor. Some of the names may occur 14 times; it is so very easy to miss one manually.

B. User-Dependent Aspects

There are some things in BLAKE that are matters of user- or installation-preference, such as the designation of input and output units.

1. The input and output units for BLAKE are named symbolically LI and LO everywhere, with three exceptions. LI and LO are set equal to 5 and 6, respectively, in the main program. The three exceptions occur in Subroutines DVDINT, MATINV, and TICTIC, where the WRITE unit is explicitly named unit 6. You may need to change these designations.

2. The program forms and then uses a binary file on unit LIB, which is set to 7 in the main program. Again, you may prefer a different number.

3. The units for input quantities in BLAKE are:

energy: calories;
temperature: Kelvins;
density: grams per cubic centimeter;
pressure: atmospheres.

These units can be readily changed by altering one or more of the constants PCON, VCON, TMCON, TACON, and HCON in the main program. These are used throughout the program as conversion factors for pressure, volume, temperature (two factors), and energy, respectively. They are now set to 1.0, 1.0, 0.0, 1.0, and 1.0.

For example, if you wanted to change input units from calories and Kelvins to joules and degrees Fahrenheit, the following changes would be made before compiling the program:

HCON = 4.184,

TMCON = 0.555556, and TACON = 255.375.

VII. USING 'BLAKE'

A. Job Control Cards and the First Two Runs

All job control cards, system cards, or their equivalent, are the responsibility of the user.

In what follows, it will be assumed that the program has been compiled and loaded without error. The very first time the program is executed, it is necessary to form the binary library that will thereafter be used in every run. Appropriate job control instructions

must be supplied to assign a file for this library, which the program assumes will be on unit 7, although you can readily change this assignment. (See Section VI.B)

The BLAKE library, which is supplied along with the program, is the input for this first run. The output produced consists of the binary library on unit 7, and a human-readable output on the chosen output device (unit 6 unless you have previously changed it). This latter output should be carefully scrutinized for error messages, which will be the first part of the output. Assuming that all of the necessary changes described in Section VI were made prior to this run, there should not be any error messages from the operating system at this point. There may, however, be error messages from the program calling attention to problems with the library. The most common one is TWO OR MORE CONSTITUENTS HAVE THE SAME NAME, which will occur if the reduction of the names of products to four or fewer characters was not done carefully.

Following the error messages (if any) will be a complete listing of the library in human-readable form. It should be painstakingly read to guard against unexpected problems (garbaged names, for example).

If it looks good, then you are ready for the second run, which will consist of the test cases also supplied with the program. Before running them, it is necessary to insert control cards that will assign the binary library formed in the previous run to unit 7.

The output from the test cases should be compared with the listing given in Appendix C of this report. Further discussion of the output is given in Section VIII.

B. Comments on the Computation of Equilibrium by TIGER

In order to shorten the discussion required for some of the instructions, a few comments are required on the philosophy of TIGER's calculation of the equilibrium state. The discussion will be entirely qualitative; the complete technical details are in the TIGER manuals⁵.

TIGER proceeds by considering at first only the gaseous constituents that are chemically-possible products of the specified mixture. Condensed phases are usually (not always) considered later if necessary. At each step the program tries to work with a set of N linearly-independent constituents that are present in the largest amounts, where N is the number of different elements present in the mixture. These N constituents are called the 'components'. Most of the computing time is spent looking for the correct set of components, which may change with conditions, (e.g., pressure or temperature) even while computing a single composition.

In theory but not in practice the program could permute all of the constituents present until it finds the components. The first attempt at finding the components consists of selecting the first linearly-independent set of constituents as they are retrieved from the library tape. This order was determined at the time the library tape was created and was based on the order of the CONStituent cards. For the elements C, H, O, and N, the components usually turn out to be CO_2 , H_2O , N_2 , and CO , which are therefore the first four constituents in the BLAKE library. See also the discussion of the instructions ORDER and ORC in Section VII C 2.

If the first selection of components proves to be wrong, the program does some permuting among the constituents. Since one knows chemically that some of the constituents will rarely if ever be present in large enough concentrations to be components, the program makes provision for skipping them. Constituents that are never to be considered as components have an asterisk (*) punched as the last field in their CONStituent instruction (See Section VII C1). When the program prints the list of constituents selected, those that cannot be components are all printed after those that will be. The dividing line between these two groups is called the 'floor'. You have the capability of raising or lowering the floor; see FLOOR in Section VII C 2).

BLAKE is presently limited to considering a maximum of 29 gaseous constituents for any one composition. Error message No. 31 is printed if more than 29 gaseous constituents are selected, and the case is rejected.

The library contains thermodynamic data for a wide range of species. Consequently, compositions with five or more elements can readily have more than 29 constituents chosen by the program and thus will not run. This potentially embarrassing problem is solved by the REJECT instruction. (See Section VII C 2).

Convergence is materially aided if you have advance knowledge of the major constituents in the equilibrium composition. Such knowledge is often obtained by running the same composition with another code. The NASA-Lewis equilibrium code is recommended for this purpose. The NOTS code used at the Naval Weapons Center also works well.

The NASA-Lewis code has the unsurpassed advantage that for a given composition, it can consider all of the chemically-possible species contained in the JANAF Tables. Thus, one can run an obstreperous formulation (one containing more than six elements) with this code first, determine the significant constituents, and then use this information to determine REJECT, ORDER, and ORC instructions for a subsequent BLAKE run.

C. General Remarks on the Instruction Set

BLAKE, like TIGER, proceeds by executing one by one a set of instructions; the BLAKE set contains 37, of which a third are truly essential, a third serve to change default values of diverse parameters, and a third are frankly frills, intended to modify, expand, contract, label, title, or comment on, the output.

To a considerable extent the actual order in which the instructions are entered by the user is immaterial. Logic, to be sure, demands that some orders precede others: a heat of explosion cannot be computed until a composition has been specified; but a title, for example, can be entered late or not at all, as you please.

The language of the descriptions of these instructions generally assumes that they are created by being typed into an input file from a terminal, but they can just as well be entered from punched cards.

Each instruction consists of a key word or abbreviation followed by a variable number of fields containing keywords or numbers. Each field is set off from its neighbors by commas. The key word or abbreviation for the instruction itself must appear in columns 1-3 of the instruction; otherwise the fields are arbitrary in both length and placement in the line.

When numbers are required in an instruction, they may be typed in free form. Thus, 69, 69., 69.0, 0.69E2, and 0.0069E04 all represent the same number in an instruction. The program decides eventually whether it needs a real number or an integer and takes appropriate action.

The general form of an instruction is:

INstruction, PAR1, n1, PAR2, n2, PAR3, n3, . . . , (PARm, nm)

Names or letters in CAPITALS must be typed just that way; no variation is permitted. Lower-case letters are added to some of the instruction names for mnemonic reasons, but are not part of the instructions name and may be omitted. Thus, FOR, FORMula, and FORMulas are all interpreted as the same instruction and all are valid. The comma marks the end of this field and separates succeeding fields from each other. In a few cases, double commas with at most blanks between them have a special significance; their use is explained in the applicable instruction.

The quantities PAR1, PAR2, PAR3, . . . , represent key words or letters and must be typed just as given for each particular instruction. The quantities 'n1', 'n2', 'n3', . . . , represent numbers that are associated with the keywords or parameters and may be typed as desired or needed.

Sometimes the parameters must appear in a specified order; othertimes order is immaterial. When the order may be varied, this is so stated; if not, assume that the items must appear in the given order.

The ellipsis, ... , indicates that a variable number of items may be entered. Names in parentheses are optional, as noted for individual instructions.

D. The Instruction Set

1. Library Instructions. The library instructions are CONStituent, ELEment, PRInt, STC, STG, STR, and END. These instructions are used to form the binary library and are understood by the program only while that operation is proceeding. This operation in turn starts with the instruction, STArT of library, which is thus not a library instruction, but which has no other purpose.

CONStituent, name, GAS, e1, n1, e2, n2, e3, n3, ...

or

CONStituent, name, CONDEN, e1, n1, e2, n2, e3, n3, ...

This library instruction defines 'name' as the official name of a constituent. One of the parameters GAS or CONDEN (for condensed) must appear. The quantities 'e1', 'e2', etc., are the symbols of the elements that appear in 'name', 'n1', 'n2', etc., are the numbers of atoms of those elements respectively. Note that a condensed constituent may appear in either the liquid state, the solid state, or both.

ELEment, sym, atwt

This library instruction defines 'sym' as the official name of an element whose atomic weight is 'atwt'. No constituent name will be accepted by the program unless all of its constituent atoms appear in ELEment instructions.

Note that if the element itself is to be allowed as a constituent, it must also appear in a CONStituent instruction.

Examples:

ELEment, NA, 22.98997

CONStituent, NA, GAS, NA, 1

If the latter instruction were omitted, then sodium could appear as NaOH or NaO, etc., but not as the monatomic gas, Na.

END of Library

This instruction marks the end of the library deck. It must appear. As soon as it is read, the program then proceeds to sort the library cards, form the binary library tape (or its equivalent on the disk), and writes the library listing (unless the latter is suppressed). Note that library instructions may appear in any order between START and END; the program sorts them after the END card has been read.

STC, name, SOLID, 1, a1, a2, a3

STC, name, SOLID, 2, a4, a5, a6

STC, name, SOLID, 3, a7, a8, a9 (and similar forms for LIQUID)

The STC instruction supplies data for the equation of state of a condensed substance, either LIQUID or SOLID. The order of the cards is immaterial, but all three must appear; if not, all of the numbers are skipped. (This will eventually lead to a run-time error, when the program tries to take the reciprocal of 'a1'.) The three coefficients must appear in the correct order on a given card, however.

The coefficients themselves belong to the empirical equation

$$V = A_1 + A_2P + a_3P^2, \quad (43)$$

where V is the molar volume of 'name', and the A_i are given by

$$A_1 = a_1 + a_2T + a_3T^2, \quad (44)$$

$$A_2 = a_4 + a_5T + a_6T^2, \text{ and} \quad (45)$$

$$A_3 = a_7 + a_8T + a_9T^2. \quad (46)$$

Here, P and T are pressure (atmospheres) and temperature (Kelvins); the a_i are represented by the 'ai' in the instruction. It is unlikely that all 9 coefficients will be known for many materials, but zeroes must appear on the cards for all missing coefficients.

STR, name, GAS, 1, b1, b2, b3

STR, name, GAS, 2, b4, b5, b6

STR, name, GAS, 3, b7, b8, b9

These instructions introduce the thermodynamic data for 'name' into the library. LIQUID or SOLID may appear instead of GAS. If a substance forms only a liquid (solid), then the instructions for solid (liquid) are omitted for that substance.

The coefficients, 'bi', are related to the heat capacity at constant pressure, C, enthalpy, H, and entropy, S, by the empirical equations

$$C = b_1 + b_2\theta + b_3\theta^2 + b_4\theta^3 + b_5/\theta + b_6/\theta^2 + b_7/\theta^3; \quad (47)$$

$$S = R(b_1 \ln(\theta) + b_2\theta + b_3\theta^2/2.0 + b_4\theta^3/3.0 - b_5/\theta - b_6/2.0\theta^2 - b_7/3.0\theta^3); \text{ and} \quad (48)$$

$$H = [RT(b_1 + \frac{b_2\theta}{2} + b_3\theta^2/3.0 + b_4\theta^3/4.0 + b_5 \ln(\theta)/\theta - b_6/\theta^2 - b_7/2.0\theta^3) + b_8 - \Delta H^\circ(298.15)]/1000.0 \quad (49)$$

Here,

$$\theta = T/1000,$$

R is the gas constant, 1.98717 cal/mole-K, and $\Delta H^\circ(298.15)$ is the standard enthalpy of formation.

These coefficients are obtained by applying least-squares techniques to suitably-selected data, preferably those in the JANAF Tables¹². BLAKE is furnished with a library containing data for 98 gases, and 22 condensed phases of 16 elements. Users desiring additional data must do their own fittings.

PRInt the Library

This instruction creates a listing of the library on output unit L0. The listing is not printed unless this instruction is entered. It may appear anywhere between STArt and END. The library listing is ordered according to the order of appearance of the CONStituent instructions and is formatted for human reference. A copy should be made every time the library is changed.

STG, name, cov, T, t, S, s

This instruction differs from the STG instruction of TIGER. Here, 'name' is the legal name of a gaseous constituent as defined by a CONStituent instruction. The quantity 'cov' is the BKW covolume of this substance (not to be confused with the covolume used in the Noble-Abel equation).

The quantities 't' and 's' are the two Lennard-Jones parameters, the well depth and the molecular diameter. The key letters T and S may be replaced by either E or D, respectively, and their order may be interchanged. Of course, 't' and 's' must be associated with the proper key letter.

It is sufficient to supply only the BKW covolume, but if one of the Lennard-Jones parameters is specified, then so must the other; if not, neither one is accepted.

2. Computational and Control Instructions. The instructions are listed in alphabetic order by their three-letter key.

CHOose, name1, name2, name3, ...

Example:

CHO, CO₂, H₂O, N₂, CO, NH₃

This instruction forces the program to consider only the named constituents as possible products of an equilibrium calculation. The names listed must be constituent names in the library. The use of this instruction is recommended only in special cases.

CM2

See the discussion under COMposition.

CMT (message)

This instruction prints the word COMMENT followed by the 'message' you have typed, all on one line. It is convenient for adding notes to the output.

Example:

CMT this is a comment card.

COMposition, name1, a1, name2, a2, name3, a3, ... , (MOLE)

This instruction defines the composition of a mixture. It is an essential instruction, as all of the computational instructions are automatically rejected if they occur before a COM instruction.

The names 'name1', 'name2', etc., must have previously been defined by FORMula instructions; otherwise, the entire instruction is rejected. The quantities a1, a2, ..., are the relative amounts of each substance. The order of the names is immaterial, but the correct amount must follow each name. The amounts need not be percentages; any basis is acceptable. Regardless of how you enter the composition, however, the program will normalize it and print it in both weight-percent and mole per cent.

If you prefer to enter your composition data in moles, the keyword MOLE must also be typed.

All of the data must fit into one 80-column line. If this is not feasible, use the instruction CM2 instead of COM. You may then extend the input data over two 80-column lines. Do not repeat CM2 at the start of the second line. The MOLE designator does not apply to CM2.

Examples:

COM, NC1325, 75, NG, 25

COMPØS, N2, 4, Ø2, 1, MØLE

DATE (message)

The separator (,) is not needed by this instruction. The date of the run is normally obtained from the operating system clock and printed on each output page. If you have trouble in obtaining this information, or if you want to print your own date, this instruction takes the last 20 characters from 'message' and prints them in place of the system date. If the 'message' is blank, the system-produced date is omitted and nothing replaces it. Once DATE has been used, you cannot return to using the system clock in the same run.

The regular use of this instruction is not recommended if you have access to the system date. The primary purpose of the instruction is to mark special days, like one's birthday, Halloween, Friday the 13th, Bandmen's Day, etc.

Example:

DAT Fourth of July

DEBug, n

If 'n' is not 0, the debug feature is turned on; if zero, it is turned off if it was on.

The 'debug' feature was taken over from TIGER, where it was introduced for assistance in developing Subroutine ECOMPO. When turned on, it prints the current temperature, pressure, volume, entropy, and energy, the current mole numbers, and the current corrections to the mole numbers on each pass through ECOMPO. In my experience it is not presently useful, and will be removed from later versions of BLAKE.

DESTroy

This instruction negates the effect of a RETain (which see) instruction.

ECHo, n

This instruction makes the program print out ('echo') each instruction as it is encountered. The feature is turned on when 'n' is non-zero, and turned off when 'n' is 0.

EXPlosion, V, vol, (EOF, e)

This instruction executes a constant-volume (isochoric) burning calculation on a previously-defined mixture. The specific volume, vol, is in cubic centimetres per gram unless you have changed the volume conversion factor (see Section IV B). Normally, the energy of formation calculated for the composition is used; if you want to use a different one, it is entered as e.

Example:

EXP, V, 5

EXl, P, p, T, t

This instruction is the same as EXP, except that it is for a gaseous mixture at pressure p and temperature t. The ideal gas law is used to calculate the volume and then EXP is called automatically. The initial energy cannot be changed.

Example:

EXl, P, 2, T, 298.15

FL0or, n

This instruction sets the level of the floor at n. See the initial discussion in Section IV. Sometimes, when you are having a lot of trouble forcing a particular computation to converge, it helps to raise the floor (that is, make n a smaller number than the program value). Sometimes it doesn't help. Once a new floor has been set, it remains at that value until either a new COM or a new FLO instruction is entered.

FORmula, name, enth, ele1, n1, ele2, n2, ele3, n3, ...

This instruction defines 'name' as the name of a reactant species; its enthalpy is 'enth' and its formula contains n1 atoms of element 'ele1', n2 atoms of 'ele2', etc. The symbols used for the elements must be exactly those that appeared on ELEment cards when the library was formed. The enthalpy of formation is entered in calories per gram-mole, not calories per 100 grams, and not kilocalories per mole.

In keeping with the TIGER and BLAKE conventions for putting numbers in instructions, the numbers n1, n2, ..., may be typed in any way. The program uses them as real numbers, so decimal fractions are accepted and used correctly. When the program goes to print the formula, however,

these numbers are converted to integer form by truncation, so that decimal fractions will not be printed properly, even though the program used them correctly. This causes trouble with polymers, since their formulas rarely contain integer numbers of atoms. It is customary for polymer compositions to be specified in units like gram-atoms per hundred grams, and with a corresponding enthalpy, but BLAKE does not accept such input data. Such data are easily converted to molecular formulas, but the numbers of atoms generally come out to be decimal fractions. This creates a small but annoying problem, since one usually prefers to have the correct formulas printed for the input. The simplest solution is to multiply the formulas and the associated enthalpy by either 1000 or 10000.

For your convenience, the formulas of many common ingredients of US propellants are stored in the program, and need not be entered on a FORMula card. The names and abbreviations of these substances are listed in Section V.

If a FORMula instruction is mistyped, or if a duplicate formula name is entered, the instruction is rejected and an error message is printed. If you wish to use a different enthalpy for a substance whose formula is prestored, you must enter a FORMula instruction for the material with a different name; the same name cannot be redefined without changing the program and then recompiling it.

A maximum of 50 additional formulas is permitted; if you try to enter more, they are rejected, and an error message is printed.

Examples:

FØR, DES, -280E3, C, 18, H, 34, Ø, 4

FØR, PG, -4E7, C, 4000, H, 5000, Ø, 100

FREEze

Most calculations are carried out with the assumption of total dynamic chemical equilibrium. The FREEze instruction 'freezes' all chemistry, so that all following calculations are done on a mixture of non-reacting gases. See also MELt.

GEO, name

Change the Gaseous Equation Of state to one of the following:

<u>Equation of State</u>	<u>Keyword</u>
ideal	IDEAL
truncated virial	VIRIAL <u>or</u> LJ
B-K-W	BKW

The default equation is the truncated virial equation. If 'name' is mistyped, the program defaults to the truncated virial.

Example:

GEO, VIRIAL

GRID, CENTER, P, np, ip, np, V, v1, nv, v2

or

GRID, CORNER, P, p1, ip, p2, V, v1, iv, v2

This instruction computes chemical equilibrium at a grid of points centered about, or cornered at, a specific point. The computations may be done for various combinations of thermodynamic variables:

pressure, volume (P, V);
pressure, entropy (P, S);
volume, temperature (V, T);
volume, energy (V, E); and
volume, entropy (V, S).

In each of these cases, the parenthesized letters are the key letters that must be used in the instruction. In all cases the order must be that given here.

The units of the extensive variables (enthalpy, energy, volume, and entropy) are specific; that is, for one gram of substance.

'p1' is the initial value of the variable (P, in this case); 'p2' is its final value. For CORNER, 'ip' and 'iv' are the sizes of the increments in those variables. For CENTER, 'np' and 'nv' are the number of increments to be inserted between initial and final values. The increments 'ip' and 'iv' may be negative if desired.

If instead of a number 'p1', 'p2', etc., a comma (with at most intervening blanks) is used, the program will automatically use the existing value of that variable. See Test Case Nine for an example.

Examples:

GRID, CORNER, P, 1, 0.1, 10, V, 20, .5, 40

GRID, CENTER, P, 1, 4, 10, V, 20, 19, 40

GUN, s, i, f

This instruction computes the thermodynamic properties of the chamber gas produced by propellant burning to equilibrium at constant volume at loading densities between s and f, at increments in loading density of i. A maximum of 16 different loading densities is permitted. If you try to use more than 16, only the first 16 are computed, and the program continues to the next instruction.

Example:

GUN, 0.05, .05, 0.40

ISOLine, T, t1, P, p1, np, p2, (LOG)

This instruction computes thermodynamic equilibrium for a set of points, one of which is held constant. In addition to temperature and pressure (as shown), the same sets of variables permitted in a GRId instruction are accepted.

The variable to be held constant is named first. 'p1' is the initial value of the variable being changed, 'np' is the number of increments, and 'p2' is the final value. If the optional parameter LOG appears, logarithmic spacing is used. Logarithmic spacing is automatically used when the variables are (S, V).

Example:

ISO, T, 1000, P, 10, 4, 20

LJP, name1, T, v1, S, v2, name2, T, v3, S, v4, ...

This instruction changes the values of the Lennard-Jones parameters for substances 'name 1', 'name 2', etc. Of course, 'name 1' must be a legal name (one that appears in the library as a CONStituent). The program checks that both parameters have been entered, even if you only wish to change one of them. Changing only one is simplified by the fact that if two successive commas with at most blanks between them appear in place of 'v1' (or 'v2', etc.) the program will use the existing value.

The order of T and S is immaterial, but 'v1' and 'v2' must correspond to the key letters used. The key letter T may be replaced by E; and S, by D.

If 'name1' is mistyped or is an illegal name, no action is taken but a diagnostic message is printed. If two or more names appear on a card and one of them is wrong, the program will nevertheless attempt to process the remaining names.

If no COMposition card has been entered, the program will reject an LJP instruction. A suitable message is printed to add insult.

Examples:

LJP, H₂O, T, 600, D. ,

LJP, NH₃, D, 4, T, 350

MELt

This instruction undoes the effect of a FREeze instruction. It, too, is optional.

ORC, name1, name2, name3, ...

This instruction is almost identical with the ORDer instruction, except for one crucial point. ORDer applies only to gaseous constituents, while ORC applies only to condensed ones. It is not often needed, but in some cases (e.g., black powder), it is quite useful.

Example:

ORC, K₂SO₄\$

ORDer, name1, name2, name3, ...

This instruction makes the program chose 'name1', 'name2', etc., as the components for the first attempt at finding the equilibrium composition. If these components are not all linearly independent, one or more of them will be omitted. The names of the constituents must be exactly the same as the names used in the CONstituent instruction when the binary library was formed. Also, none of these substances may have been previously rejected by a REject instruction. If either of these conditions is violated, the entire case is omitted and the program continues.

Example:

ORD, N₂, H₂O, CO₂

POInt, P, p, T, t

This instruction computes chemical equilibrium at the point with the specified pressure 'p' and the specified temperature 't'. The order in which they appear is not arbitrary; it must be (P,T), (P,V), (P,H), (P,S), (V,E), (V,T), or (V,S). If the wrong order is used, an error message is printed and the program proceeds to the next case.

Example:

POINT, P, 10, T, 2500

PRLimit, CON, v1, FIT, v2, ERR, v3, PAG, v4

This instruction controls the amount of output printed by BLAKE. The order of the keywords is immaterial but they must be typed or punched just as shown. (For example, do not use 'PAGE' for 'PAG'.) The numbers 'v1', 'v2', ..., are either 0, 1, or 2, and have the following significance:

CON, 2: Print the list of constants for the fitting of the thermodynamic data of each constituent. This list is printed once after a COMposition instruction is entered provided PRL, CON, 2 has been specified. The list is not repeated until another PRL, CON, 2 instruction is given. Instead the program reverts to PRL, CON, 1.

CON, 1: This is the default setting. The list of constants is not printed but the composition of the chamber gas is printed after each GUN instruction. PRL, CON, 2 reverts to this setting.

CON, 0: The printing of both the constants and the composition of the chamber gas is suppressed. Once set, this instruction remains in effect until changed.

FIT, 1: Fit the four quantities, chamber pressure and temperature, and covolume and gamma of the chamber gas, to a cubic polynomial in the loading density. The fitting is done provided at least four loading densities are called for in the GUN instruction.

FIT, 0: Suppress the fitting, no matter how many loading densities are called for. Once entered, this instruction remains in effect until changed. This is the default setting.

PAG, 1: Put each distinct part of the output from a GUN instruction on a separate page. These parts are the composition (including the list of thermodynamic constants if called for), the thermodynamic functions for the chamber gas, and the summary. This is the default setting. Each output page produced has its own title (if one was entered), the date (either from the system or from a DATE instruction), and the version designator.

PRL, 0: Do not paginate the output until a page is filled, or until a new COMposition instruction is entered.

ERR, 1: Print each occurrence of error messages 28 and 30 as they occur.

ERR, 0: Suppress the printing of these error messages. A summary of the total number of occurrences of each error is printed at the end of the case. This is the default setting.

Not all of the parameters on a PRL instruction need be specified at once; you need only include the one(s) you want changed.

Examples:

PRL, CON, 0

PRL, CON, 0, PAG. 0

PRL, CON, 2, FIT, 1

QEXplosion, R, r, T, t

This instruction computes the heat of explosion of a composition at loading density 'r' at five freeze-out temperatures centered around temperature 't'.

The composition must have been entered previously. The order of 'r' and 't' is unimportant, but the values entered for 'r' and 't' must correspond to their key letters.

The five temperatures are $t - 200$, $t - 100$, t , $t + 100$, and $t + 200$.

The algorithm used is that of Corner¹. The program executes a POInt computation at the volume $1/r$ and the chosen temperatures.

The working of the algorithm is critically dependent upon the contents of two DATA statements in the subroutine that contain the names and enthalpies of formation of stable final products at 298 K. This list has been selected for compounds formed by the elements carbon, hydrogen, nitrogen, oxygen, boron, potassium, and sulfur. If additional elements are present in a given formulation, appropriate changes must be made to the DATA statements. Version 205.0 allows room for seven additional compounds without other programming changes being required.

Example:

QEXP, R, 0.2, T, 1100

QUIt

This instruction should be the final one in every BLAKE run. It causes the program to execute a normal FORTRAN STOP. If it is omitted, the program will likely stop because it will next read an end-of-file. Using the QUIT instruction is more elegant.

RECall, name1

Example:

RECALL, NUM1

This instruction recalls the final conditions associated with the state designated by 'name1'. If the point has not been saved (see SAVE), an error message is printed, and succeeding calculations are either skipped or done erroneously, until a new COMposition instruction is entered.

REJect, name1, name2, name3, ...

This instruction eliminates from further consideration the constituents whose legal names are 'name1', 'name2', etc. If an illegal or undefined name is entered, it is ignored without harm. See also DESTroy and RETain. The maximum number of constituents that may be REJected is 99.

Example:

REJ, C(s), C₂H, C₂N, C, CH

RETain

This instruction causes the program to retain a list of REJects from one COMposition to another. If it is not used, an existing REJect list is automatically cancelled when a new COMposition instruction is entered. The effect of RETain is negated by DESTroy.

SAVE, name

BLAKE and TIGER start new thermodynamic calculations from the results of a previous one, except when initialized by a COMposition instruction. Then the program starts from a pre-set guess that may be far from the final composition. The convergence of a calculation can often be made more efficient by having the program start from the results of an earlier calculation. This intent must be made known in advance by use using the SAVE instruction. The conditions (including the final concentrations) just computed are saved in memory, and the name 'name' is associated with them. Up to 8 points may be saved in this way, and later recalled (see RECall). If you try to save more than 8, an error message is printed, and the point is not saved. A name may be reused, however, the new point will then overwrite the old one.

Example:

SAV, NUM1

STArt the Library

This instruction is used to form the binary library. See Section VI A.

TITle, (message)

This instruction causes a title to be written at the top of each page of output. All of the characters in 'message' are centered and printed.

Example:

TIT, THIS IS A TITLE

TIME, t

This instruction is system-dependent (see Section VAl). If you have implemented it on your system, then it is used to change the default setting of the maximum time allowed for a single calculation by BLAKE. It is useful in the case that you want to run a number of different cases that you anticipate will require a maximum of (say) five minutes. It is unlikely that you will want all five minutes to be devoted to one case. By setting the TIME instruction, you can control approximately the amount of time the program devotes to one case before going on to the next. This time limit is different from, and independent of, the time limit that is usually set at the beginning of a run by your job card (or other job control entry).

This instruction is optional. If you have implemented the CLOCK instructions, you can then set a default time limit. For the UNIVAC 1108, 2.5 minutes was a reasonable value; for the CDC 7600, 0.4 minutes is better.

The actual time that elapses before time is called by this instruction is usually greater than the value set, because the program only checks the clock at certain cycle limits.

Example:

TIM, 0.1

TRAnsport properties

This instruction is inactive. Someday it will cause the program to compute approximate values for viscosity and thermal conductivity. Some day gold will fall from the sky.

UNIts, name

This instruction causes the program to include or exclude English (or conventional engineering) units for the summary output in a GUN

calculation. The summary output is always printed in SI units. This cannot be suppressed except by changing the program. If in addition, you want English units printed, this instruction will do that when 'name' is ENG. If 'name' is 'SI', the English unit print is suppressed.

Example:

UNI, ENG

E. Error Messages

There are two score plus four error messages contained in BLAKE. Only a few of them (e.g., types 9 and 24) indicate truly serious problems and terminate a case. Most of the others call your attention to situations that may need corrective action, but the program continues with the same case. A few indicate that the program is having problems reaching equilibrium. Where appropriate the program prints the instruction that is the source of a problem.

All of the error messages incorporated in the code are listed here. (Some of the error messages of TIGER were removed, hence the gaps in the numbering.) The exact message is listed IN CAPITAL LETTERS; then the probable cause is discussed and remedial action suggested.

Error Type 1: INPUT CARD NOT ACCEPTABLE.

The instruction entered is not one of the 37 recognized by BLAKE. The instruction is skipped and the program attempts to interpret and follow the next instruction. This message usually arises from faulty typing or punching.

Error Type 2: TOO MANY CONSTITUENTS REJECTED.

Since up to 99 constituents may be rejected, this message is very improbable. It could occur towards the end of a very long run in which you forgot to DESTory several previous REJect lists; even this is improbable.

Error Type 3: TOO MANY CONSTITUENTS ORDERED.

Only 25 constitutents may be ordered. The program continues but only the first 25 constituents are ordered. There is never any need to order as many as 10 constituents; one per element is sufficient.

Error Type 4: TOO MANY CONSTITUENTS CHOSEN.

The limit is 25. The program continues but only the first 25 constituents are chosen. Again, there is little reason for trying to choose 26 or more constituents. As mentioned earlier, this order is better not used.

Error Type 6: FINDING RHO EXCESSIVE ITERATIONS.

This error message arises in Subroutine FINDRH; PO and P are printed at the same time. When $P = PO$, a value for RHO has been found, so the difference between the two is a measure of the error at that time. The program uses the last value of RHO and continues. If it converges later, this error can be safely ignored.

Error Type 7: FINDING TO EXCESSIVE ITERATIONS.

This message arises in Subroutine FINDTP; PO and P are printed at the same time. When these two are equal, a value for TO has been found so their difference indicates the magnitude of the error. The program uses the last value of TO and continues. If it later converges, this message can be ignored.

Error Type 8: COMPONENTS LINEARLY DEPENDENT.

This message arises in Subroutine SELECT. It usually means that you have CHOsen constituents unwisely or have been unlucky with an ORDER instruction. REJect a condensed constituent and try it again.

Error Type 9: NO ACCEPTABLE COMPONENTS.

This is one of the most frustrating messages of all. It arises in Subroutine SELECT and indicates that the program cannot find a set of linearly independent components after trying many sets above the floor. The case is rejected and the program continues. Unfortunately it does not give a list of the constituents it has considered nor the position of the floor. There is no certain procedure to follow at this point. I usually add another REJect list, play with an ORDER or ORC instruction, or as the last resort, raise the floor.

Error Type 11: EXPLOSION STATE CARD NOT ACCEPTABLE.

This message arises in Subroutine EXPLOS. It indicates that either an EXPlosion or E/X instruction has been incorrectly punched. The offending instruction is printed to facilitate the detection of the error. The case is rejected and the program continues.

Error Type 12: INPUT TO POINT NOT ACCEPTABLE.

This message arises in Subroutine POINNT. It indicates that an error has been made on either a POInt, ISoline, or GRId instruction. Generally this means that the variables were ordered incorrectly; e.g., V, P instead of P, V. The instruction is rejected and the program continues.

Error Type 13: THIS POINT NOT SAVED.

This message is printed in Subroutine RECALL and is self-explanatory. Usually it arises from a punching or typing error. It can also occur when a previous case was rejected or failed to converge, so the point that was to have been saved was not computed. The program continues with the succeeding instruction. The remedy is obvious.

Error Type 14: TOO MANY POINTS SAVED.

This message arises in Subroutine SAVE and is self-explanatory. The limit is eight. The point is not saved, the program continues, and will probably soon come to grief when you try to RECALL the unsaved point. The remedy is obvious.

Error Type 16: LIBRARY CARD NOT ACCEPTABLE.

This message arises in Subroutine LIBRARY. It indicates that a library instruction has failed to pass all of the checks built into the program. The instruction is printed; it should be compared with the prescribed format for library instructions. Punching or typing errors are the most common causes. The program ignores the bad instruction and continues, but you probably will not want to use the library thus formed. The binary library cannot be corrected; it must be formed all at once. Fix the card and start again.

Error Type 17: COMPOSITION CARD NOT ACCEPTABLE.

This message arises in Subroutine COMPOS. Its most common cause is that a formula card was either omitted entirely, or that it was previously rejected by the program. Punching or typing errors are the next most common causes. The offending card or instruction is printed. The program ignores the instruction and tries to continue since later COMPOSITION instructions may be acceptable. The remedy is obvious.

Error Type 19: FORMULA ELEMENTS NOT IN LIBRARY.

This message arises in Subroutine FORMULA, and is self-explanatory. The program ignores the instruction and continues. If not due to a mere typing blunder, this error is difficult to fix, since it involves adding another element to the library, a time-consuming job.

Error Type 20: NOT ALL ORDERED CONSTITUENTS IN LIBRARY.

This message arises in Subroutine COMPOS. It is caused by the listing on an ORDER or ORC instruction of a constituent that the program cannot find in the binary library. Typing or punching errors are the first thing to look for, but an equally likely error is that the substance in question had been previously listed in a REJECT instruction. The program

ignores the instruction, rejects the case, and continues. The remedy is obvious although it is not always easy to decide which constituent in an ORDER or ORC instruction was at fault.

Error Types 21, 22 and 23: FREEZE MATRIX SINGULAR.
FREEZE FORCE ITERATION EXCEEDED.
FREEZE ITERATION EXCEEDED.

All of these messages arise in Subroutine FREEZE. All three errors are fatal to the computation being attempted. The program skips it and looks for a new COMposition instruction. The usual causes are either the frozen composition requested cannot exist at the point requested, or the point in question is too far from the last computed point.

Error Type 24: THERMO ITERATION EXCEEDED.

This message arises in Subroutine THERMO and is fatal. The program continues and looks for a new COMposition instruction. The most common cause is that it was not working with a good set of components. (Read Section VIIA over). The only cure is to use ORDER or ORC instructions to rearrange the order in which components are selected, or to change the REject instructions, or both. It is worth trying extreme measures to make a calculation converge somehow; once it has, that point can be SAVED and used to restart a new calculation with fewer restrictions.

Error Type 25: MELTING TEMPERATURE EXCESSIVE ITERATIONS.

This message arises in Subroutine ECOMPO. It is not a fatal error but indicates that the program is having some difficulty converging. Keep in mind that the version of TIGER on which BLAKE is based often encountered insurmountable problems when it tried to deal with a constituent in the neighborhood of its melting point. The new TIGER handles such computations with ease. If the computation you are trying eventually converges, fine; otherwise it is beyond BLAKE's capabilities.

Error Type 26: ECOMPO FORCE EXCESSIVE ITERATIONS.

This is a non-fatal error arising in Subroutine ECOMPO. It indicates that the program is having trouble converging. If it eventually does converge there is no problem; if not, you will get a different message (usually No. 24).

Error Type 27: SOLVING FOR ETAS MATRIX SINGULAR.

See No. 26.

Error Type 28: SOLVING FOR ETAS EXCESSIVE ITERATIONS.

See No. 26.

Error Type 29: SOLVING FOR N(I)S MATRIX SINGULAR.

See No. 26.

Error Type 30: SOLVING FOR N(I)S EXCESSIVE ITERATIONS.

See No. 26. Messages 28 and 30 are often produced during the course of a straightforward computation that converges in a few more iterations. For this reason BLAKE generally suppresses their printing. If you want to see them, use the instruction, PRL, ERR, 1. Note that even if they are suppressed, a summary of the number of times each was encountered is still printed.

It is of course possible to make the appearance of all these error messages less likely by raising the limits of the iteration counters set in the main program. I have played this game occasionally, but while it always used up more computer time, it rarely helped with a difficult computation.

Error Type 31: TOO MANY GASEOUS CONSTITUENTS.

This message arises in Subroutine COMPOS, and indicates that more than 29 gaseous constituents have been selected from the binary library. It does not tell you which 29 they were but you can readily work this out for yourself by reference to a library print. The program skips this case and continues looking for a new COMposition instruction. The only cure is to add more REjects.

Error Type 32: TOO MANY CONDENSED CONSTITUENTS.

The limit here is 10, but experience shows that the program will not converge when more than four condensed constituents have been selected. With the library furnished with BLAKE this error can arise only if you try compositions with at least nine elements.

Error Types 33 - 37: TOO MANY (....) CARDS.

All of these errors arise in Subroutine LIBRARY and are self-explanatory. The ellipsis can be filled with ELEMENTS, CONSTITUENTS, STG, STR, or STC. The limits presently set in the program are:

ELements: 40

CONstituents: 180

STG: 99

STR: 540

STC: 180

Any of these errors can be readily avoided by redimensioning the appropriate array in Subroutine LIBRAY. If you do, remember to change the error messages accordingly. (This is not absolutely necessary, of course; it is likely that the error message will be encountered by someone else who will have no idea that it is meaningless. As booby traps go, this is a relatively harmless one.)

The last six error messages unnumbered:

TWO OR MORE (...) HAVE THE SAME NAME

The ellipsis can be either ELEMENTS or CONSTITUENTS. Both messages arise in Subroutine LIBRAY and are self-explanatory. If you had to limit the length of a name to four characters (see Section VI A3), you will surely see this message unless you have scrupulously examined the library before attempting to form the binary library file for the first time. The remedy is obvious.

LJP CARD IS FAULTY OR PREMATURE.

This message arises in Subroutine LJCH and is self-explanatory. The program skips the instruction and proceeds.

---DOES NOT APPEAR IN THE LIST OF GASEOUS CONSTITUENTS

The dash is filled by the name of a putative constituent from a LJP instruction (see Section VII C2). The meaning is self-explanatory. The program skips the instruction and proceeds.

NO COMP CARD, NO CALCULATION

This message arises in Subroutine QEXP and is self-explanatory. The program skips the instruction and proceeds.

CALCULATION REJECTED

This message arises in Subroutine REJECT. When either fatal error 9 or 24 is encountered, the program prints the appropriate error message and then branches to Subroutine REJECT where various counters are reset and this message is printed. The program then proceeds, but almost all further instructions are skipped until a new COMposition instruction is found. Only TITle and QUIt are recognized.

It is hard to give good advice at this point; however, see the discussion for Error Types 9 and 24.

UNITS CARD IS FAULTY. NOTHING DONE.

This message arises in the main program and is self-explanatory. Only ENG or SI are recognized keywords in a UNITS instruction. The program proceeds.

GEO CARD IS FAULTY.

This message arises in the main program. Only IDEAL, L-J, BKW, and VIRIAL are recognized keywords on a GEO card. If a faulty card is entered, the program reverts to the truncated virial equation of state, and then proceeds.

ILLEGAL INPUT FOR CJPREP. OMITTED.

This message arises in Subroutine CJPREP and indicates that an error was made on an EX1 instruction. The instruction is skipped and the program proceeds with the next instruction.

TIME HAS BEEN CALLED. RETURN TO START. DO NOT PASS 'GO'. DO NOT COLLECT TWO HUNDRED DOLLARS.

As mentioned in Section VI A1, the program contains the capability of timing a calculation independent of the total time allowed for the entire run, provided you have implemented the call to the system clock. This message is printed if the allotted time is exceeded. There are few calculations that will converge in a longer time if the default time is appropriate to your computer. (The BRL's experience has been that 0.4 minute is a suitable limit for the CDC 7600, and 2 minutes for a UNIVAC 1108. A few extra lines of programming will readily enable you to print out the elapsed time per run if you have previously implemented the call to the system clock.)

Rather than setting a longer time limit (using the instruction TIME, t), you should fiddle with the ORDER and REJECT instructions to try to make the calculation converge more rapidly.

DUPLICATE FORMULA CARD -- IGNORED.

This message arises in Subroutine FORMLA; it is followed by a listing of the duplicate card in question. It means that you have entered a FORMULA card using a reserved name on the prestored list. The program checks only on the name, not on the enthalpy. If you want to use a different enthalpy for a pre-stored formula, you must insert a new FORMULA card with a different name.

BAD FORMULA CARD -- EITHER TOO MANY OF THEM OR THE CARD IS MIS-PUNCHED.

This message arises in Subroutine FORMLA and is self-explanatory. In checking to see why the program has declared a card to be mis-punched, pay particular attention to the difference between letter O and numeral

0. In any case the offending card is skipped and the program proceeds. Soon afterwards, you will likely get Error Type 17. Such is life.

ERROR. GUN CARD HAS MIS-FIRED.

This message arises in Subroutine GUNCAL and means that a GUN instruction is faulty. The program skips it and proceeds.

AN 'EOF' HAS BEEN ENCOUNTERED. EXECUTION TERMINATED.

This message arises in Subroutine CARDRD. On CDC computers it prevents the program from aborting when it tries to read an end-of-file, thus saving a page of incomprehensible printing. You can always end the program this way but it is suggested that you enter a QUIT instruction instead.

These 44 messages are the total embedded in BLAKE; any others must have come from your operating system.

VIII. THE OUTPUT FROM 'BLAKE'

Appendix C contains the output produced by the BRL's CYBER system for nine different BLAKE runs. They are included here both for their didactic value and as comparisons for users to ensure that their computers are producing the same numbers. In making such comparisons bear in mind that agreement for the last digit is not to be expected; discrepancies of up to a few tenths of a percent can be expected from rounding errors.

The ECHO feature was used in all of these runs to show the instructions entered. Special attention should be given to the REJECT, ORDER, and ORC instructions since these potentially offer the most difficulty for users.

The output starts with a banner page identifying the version number and proclaiming BLAKE's relation to the TIGER program. The date is printed next (assuming either that the system function DATE was implemented, or that a DATE instruction was used).

If either a CMT or ECHO instruction was entered, their output comes on the same page; neither of these instructions ever generates a page eject.

A COMposition instruction always produces a page eject. The automatic page numbering starts with this next page; it cannot be suppressed or re-started within a run. If a TITLE instruction was entered, the title (centered) is printed. Then comes the standard heading, THE COMPOSITION IS, which is followed by a listing of the ingredients specified in the COMposition instruction.

Each ingredient is followed by its weight and mole percent in the formulation, its enthalpy of formation, and its formula. In the test cases, note that most of the ingredients are those already stored in the program, and are called up by using the proper abbreviation. One exception occurs in the test case two where it was desired to use potassium cryolite as an ingredient instead of sodium cryolite. The latter is stored in the program under the name CRY; potassium cryolite must therefore be given a different name (KCRY, in this case).

The program next prints the heat of formation of the composition on both specific (per gram) and molar bases. (Owing to the form of the formulas used for nitrocellulose and other polymers, their mole fractions are distorted; likewise, the molar heat of formation of the formulation is rarely meaningful.

Then the program prints the ultimate elemental composition of the formulation in mole percent.

A page eject normally occurs at this point unless it has been suppressed by a PRL, PAG, O instruction. (See, for example, the output for test case 5.) If the list of possible products has been requested (by a PRL, CON, 2 instruction), it is now printed. See page 2 of the output for test case one.

After the standard heading and title (if any) are printed, the program prints the thermodynamic constants for the gaseous constituents of possible products. Not all of these may ultimately appear in the final equilibrium composition, but no others will be considered. The ordering is the one in which these constituents appear in the binary library unless an ORDER or CHOose instruction has been used.

The information printed for each constituent is as follows. The formula of the constituent (as defined previously on a CONStituent card when the binary library was formed), the BKW covolume, the two Lennard-Jones force constants, and then the 9 constants that reproduce the various thermodynamic properties of the constituent as a function of temperature. (See the discussion in Section VII C1, under STR.)

The floor (see Section VII A) is printed.

If any condensed constituents have been selected, their thermodynamic data are printed next. Owing to the length of the names of some of the condensed species, some arbitrary truncation had to be imposed on them. The correct formulas are printed in the listing produced when the library is first formed. This is the explanation of the cryptic message FRMS IN LIB PRT that next appears. The symbols B and C are the coefficients for the thermodynamic data and the equation of state data for the condensed species. (See STR and STC in Section VII C1.) As noted on the print, the data are arranged in the order thermo data for liquid, then solid, and

p-V-T data for liquid, then solid. If the species in question does not form a liquid (solid) phase, only zeroes appear for the liquid (solid) line.

The next part of the output depends on the computation selected. If the printing of the final equilibrium composition has not been suppressed, it comes next. The order is now different from that in which the thermodynamic constants were printed; it is essentially that of decreasing concentration. The concentration unit printed is moles per kilogram of starting materials which has proved the most convenient for users. The program prints the concentrations of all gaseous species first followed by the concentrations of condensed species; then it prints the total moles of gas. Eventually the total grams of condensed-phase material will be printed but this is not now done in version 205.0.

For a GUN instruction the program next prints a summary, the output of most interest to ballisticians. This summary presents the properties of the chamber gas at equilibrium for each loading density specified in the GUN instruction. These properties are the pressure, temperature, impetus, molecular weight of the gas, covolume, gamma, heat capacity at constant pressure, the second and third virial coefficients, the specific gas volume, and also the entropy, enthalpy, internal energy, adiabatic exponent, and compressibility.

Most of these quantities are self-explanatory. If no condensed phase has formed then the specific gas volume is exactly the reciprocal of the loading density; if, however, some condensed material has formed, BLAKE subtracts its volume from the total (geometrical) volume and prints the remainder. It is this remaining volume that is printed under the heading, GAS VOL.

Likewise, the heading MOL WT GAS indicates that the number there printed refers to the gas phase only. This point should be kept in mind when comparing BLAKE output with that produced by CEC71, where the molecular weight printed is for the entire equilibrium mixture. Also, this correction carries over to the IMPETUS, which in BLAKE is computed strictly for the gas phase only.

The heat capacity and the gamma printed are computed with the assumption that the chemical composition of the mixture is fixed, or 'frozen.' The equilibrium heat capacity is larger, since it contains the frozen term plus a contribution arising from the effect of temperature on the shifting equilibrium. This same effect makes the equilibrium gamma smaller. The difference is quite noticeable for hot propellants like M9. The matter is discussed in more detail by several writers; see, for example, a paper by Fifer and Cohen²⁴. BLAKE prints only the frozen

²⁴R. A. Fifer and A. Cohen, "High Temperature Thermal Conductivity and Heat Transfer in Gun Propellant and Primer Combustion Gases," Proceedings of the XIV JANNAF Combustion Meeting.

quantities since these are the ones that have been traditionally used in ballistic performance codes. Whether this is correct or not, and the size of the error thus introduced if it is not, remain open questions.

The adiabatic exponent is the true equilibrium derivative $-(\partial \ln P / \partial \ln P)_s$.

The quantity ϕ that is printed last is the ratio of the non-ideal pressure to the ideal pressure. It is thus a measure of the deviation of the system from ideality. The theory on which the gas pressure correction is based may not be valid for ϕ much greater than 1.5.

If the instruction UNIts, ENG, has been entered, the program now repeats the summary, this time using the proscribed units, pounds mass, pounds force, pounds per square inch, cubic inches, etc.

If four or more loading densities have been requested and if a PRL, FIT, 1 instruction has been entered, the next part of the output consists of coefficients. These coefficients are for cubic polynomials whose independent variable is the loading density. They are printed in order of increasing power from 0 to 3. The quantities fitted are the impetus, chamber pressure, chamber temperature, and covolume. The coefficients are obtained by a least-squares process and are useful from the lowest density up to the largest density fitted. They should not be used for even short extrapolations.

Test cases six, seven, and eight are further examples of the use of BLAKE for GUN calculations. Note the variations produced by the use of different PRL instructions. These cases also give interesting examples of the application of the instructions ORDer, REJect, and ORC.

Test case nine shows a different calculation that is sometimes useful. A typical double-base propellant is first allowed to reach equilibrium at a constant volume of 5 cc/g; the resulting hot gas is then expanded adiabatically. A PRL instruction is used to control the printing of the constituents.

The expansion calculation is ordered by the instruction

ISOline, S, , V, 5, 7, 500

Note the double , , ; this instructs the program to use the value of entropy previously computed, a number the user does not know in advance.

The output in this case is mainly self-explanatory. ALPHA and BETA printed here are, respectively, the quantities $\frac{1}{p} \frac{\partial e}{\partial v}$ and $\frac{1}{v} \frac{\partial e}{\partial p}$ v.

SIGMA is the Riemann integral, $-\int_{a_1}^{a_2} c_1 da$

where c_1 = local sound speed, and

$$a = \log v$$

OMEGA is the integral

$$- \int_{a_1}^{a_2} c_1^2 da$$

IX. ACKNOWLEDGMENTS

So many people from the Interior Ballistics Division have contributed or assisted with the development and improvement of the program that the naming of names presents the danger of causing hurt by omission. But it would be churlish to use this as an excuse not to try. May the omissions be few, and those, the forgiving ones.

My introduction to the need for and complexities of thermodynamic computations on real propellants came from Paul G. Baer, the co-author of BRL 1338 and of the Baer-Fortman code. It is noteworthy that Paul, an insightful modeller, is also a model of insight which he is always willing to share.

Ingo May has been an enthusiastic supporter of BLAKE from the beginning and suggested several significant improvements, especially the pre-stored formulas. This report would not yet be written without his friendly and unflagging encouragement.

R. D. "Andy" Anderson has borne the burden of the systems programming for the last six or seven years, and has guided BLAKE from BRLESC to the UNIVAC to the present CYBER. The useful instruction ORC could not have been implemented without his methodical forays into the code.

Kevin White has never been directly involved with BLAKE, but his persistent quest for molecular interpretations forced me to a deeper understanding than would otherwise have existed. My orientation is still 19th-century, but he changed my allegiance from Duhem to Boltzmann.

Last but not least, I want to express my appreciation to the authors of the original TIGER code, especially William Zwisler, for their forbearance and toleration while TIGER metamorphosed into BLAKE.

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APPENDIX A.

COMPOSITIONS OF PROPELLANTS USED IN COMPARISON CALCULATIONS

71/72

APPENDIX A

COMPOSITIONS OF PROPELLANTS USED IN COMPARISON CALCULATIONS

I. Crow-Grimshaw

Designation:	<u>N(1)</u>	<u>N(2)</u>	<u>N(3)</u>	<u>C(1)</u>	<u>C(2)</u>	<u>C(3)</u>	<u>B(1)</u>	<u>B(2)</u>	<u>B(3)</u>
<u>Ingredient</u>									
NC1260	97.10	96.9	94.8	---	---	---	40.43	40.49	40.57
Diphenylamine	0.47	0.46	0.45	---	---	---	---	---	---
Acetone	---	2.14	4.25	.23	1.17	2.3	.17	.16	.17
Nitroglycerin	---	---	---	28.74	28.67	28.79	59.40	59.35	59.26
NC1320	---	---	---	71.03	70.16	63.91	---	---	---
Water	2.43	0.5	0.5	---	---	---	---	---	---

APPENDIX A

COMPOSITIONS OF PROPELLANTS USED IN COMPARISON CALCULATIONS

II. Vest

Designation:	<u>Type I</u>	<u>Type II</u>
<u>Ingredient</u>		
NC 1313	83.25	---
Nitroglycerin	10.29	20.49
Dibutylphthalate	5.14	---
Diphenylamine	1.01	0.70
Water	0.31	0.41
NC 1323	---	78.46
Dinitrotoluene	---	0.97
Potassium nitrate	---	0.94
Barium nitrate	---	1.36
Graphite	---	0.27

APPENDIX B
FORMULAS OF INCREDIENTS PRESTORED IN 'BLAKE'

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
ACETON	-.59270E+05	58.0804	C H O 3 6 1
ETOH	-.66420E+05	46.0694	C H O 2 6 1
EC	-.25100E+05	268.3598	C H O N 17 20 1 2
NDPA	.15400E+05	214.2242	C H O N 12 10 2 2
NNDP	.54000E+04	259.2217	C H O N 12 9 4 3
NG	-.88600E+05	227.0872	C H O N 3 5 9 3
NQ	-.22100E+05	104.0686	C H O N 1 4 2 4
DNT	-.17100E+05	182.1360	C H O N 7 6 4 2
DBP	-.20140E+06	278.3496	C H O 16 22 4
ALC	-.66420E+05	46.0694	C H O 2 6 1
KS	-.34266E+06	174.2536	K S O 2 1 4
CRY	-.78900E+06	209.9413	NA AL F 3 1 6
KN	-.11776E+06	101.1029	K N O 1 1 3
BANITR	-.23706E+06	261.3498	BA N O 1 2 6
DPA	.31070E+05	169.2267	C N H 12 1 11
H2O	-.68315E+05	18.0154	H O 2 1
C	0.	12.0110	C 1

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
KBF ₄	-.45100E+06	125.9016	K B F 1 1 4
PETN	-.12880E+06	316.1386	C H O N 5 8 12 4
RDX	.14690E+05	222.1176	C H N O 3 6 6 6
AMYLPH	-.22090E+06	306.4036	C H O 18 26 4
N ₂	-.59300E+03	28.0134	N 2
N ₂ H ₄	.22750E+05	32.0454	N H 2 4
AKAR2	-.25500E+05	226.2790	C H N O 14 14 2 1
IPAN	-.96400E+05	122.1250	C H O N 3 10 3 2
HNO ₃	-.41610E+05	63.0129	H N O 1 1 3
PBO	-.10350E+06	223.1994	PB O 1 1
DEGDN	-.10350E+06	196.1172	C H N O 4 8 2 7
AN	-.87370E+05	80.0432	N H O 2 4 3
MC	-.17500E+05	240.3058	C H N O 15 16 2 1
HAN	-.87600E+05	96.0430	N H O 2 4 4
TATB	-.33400E+05	222.1170	C H N O 3 6 6 6
GLY	-.15978E+06	92.0944	C H O 3 8 3
EGLY	-.10873E+06	62.0688	C H O 2 6 2

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
CEDAC	-.32300E+08	24265.0000	C ⁹⁸³ H ¹³⁸³ O ⁶⁹²
O2	-.59300E+03	31.9988	O ²
CETAC	-.37340E+08	28376.0000	C ¹¹⁷⁹ H ¹⁵⁷⁹ O ⁷⁸⁹
TEGDN	-.13850E+06	240.1710	C ⁶ H ¹² N ² O ⁸
BAO	-.13100E+06	153.3394	BA ¹ O ¹
METRID	-.10600E+06	255.1420	C ⁵ H ⁹ N ³ O ⁹
ETHER	-.66750E+05	74.1234	C ⁴ H ¹⁰ O ¹
TMAN	-.74100E+05	122.1246	C ³ H ¹⁰ N ² O ³
PB2CO4	-.21950E+06	490.4086	PB ² C ¹ O ⁴
DECA	-.55120E+05	138.2522	C ¹⁰ H ¹⁸
EDDN	-.15620E+06	186.1242	C ² H ¹⁰ N ⁴ O ⁶
HN	-.60130E+05	95.0578	N ³ H ⁵ O ³
UDMH	-.12690E+05	60.0986	C ² H ⁸ N ²
EOAN	-.12360E+06	124.0962	C ² H ⁸ N ² O ⁴
TRIAC	-.28018E+06	218.2070	C ⁹ H ¹⁴ O ⁶
HMX	.17900E+05	296.1560	C ⁴ H ⁸ O ⁸ N ⁸
NC1100	-.18086E+09	250754.5000	C ⁶⁰⁰⁰ H ⁸⁰³¹ O ⁸⁹³⁹ N ¹⁹⁶⁹

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1101	-.18079E+09	250879.1000	C H O N 6000 8028 8944 1972
NC1102	-.18072E+09	251003.9000	C H O N 6000 8025 8950 1975
NC1103	-.18066E+09	251128.8000	C H O N 6000 8022 8955 1978
NC1104	-.18059E+09	251253.8000	C H O N 6000 8020 8961 1980
NC1105	-.18052E+09	251378.9000	C H O N 6000 8017 8966 1983
NC1106	-.18045E+09	251504.2000	C H O N 6000 8014 8972 1986
NC1107	-.18038E+09	251629.6000	C H O N 6000 8011 8977 1989
NC1108	-.18032E+09	251755.1000	C H O N 6000 8008 8983 1992
NC1109	-.18025E+09	251880.8000	C H O N 6000 8006 8989 1994
NC1110	-.18018E+09	252006.5000	C H O N 6000 8003 8994 1997
NC1111	-.18011E+09	252132.4000	C H O N 6000 8000 9000 2000
NC1112	-.18005E+09	252258.4000	C H O N 6000 7997 9005 2003
NC1113	-.17998E+09	252384.6000	C H O N 6000 7995 9011 2005
NC1114	-.17991E+09	252510.9000	C H O N 6000 7992 9017 2008
NC1115	-.17984E+09	252637.2000	C H O N 6000 7989 9022 2011
NC1116	-.17977E+09	252763.8000	C H O N 6000 7986 9028 2014
NC1117	-.17970E+09	252890.4000	C H O N 6000 7983 9033 2017

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1118	-.17964E+09	253017.2000	C H O N 6000 7980 9039 2020
NC1119	-.17957E+09	253144.1000	C H O N 6000 7978 9045 2022
NC1120	-.17950E+09	253271.1000	C H O N 6000 7975 9050 2025
NC1121	-.17943E+09	253398.3000	C H O N 6000 7972 9056 2028
NC1122	-.17936E+09	253525.6000	C H O N 6000 7969 9062 2031
NC1123	-.17929E+09	253653.0000	C H O N 6000 7966 9067 2034
NC1124	-.17922E+09	253780.5000	C H O N 6000 7963 9073 2037
NC1125	-.17915E+09	253908.2000	C H O N 6000 7961 9079 2039
NC1126	-.17908E+09	254036.0000	C H O N 6000 7958 9084 2042
NC1127	-.17902E+09	254163.9000	C H O N 6000 7955 9090 2045
NC1128	-.17895E+09	254292.0000	C H O N 6000 7952 9096 2048
NC1129	-.17888E+09	254420.2000	C H O N 6000 7949 9101 2051
NC1130	-.17881E+09	254548.5000	C H O N 6000 7946 9107 2054
NC1131	-.17874E+09	254676.9000	C H O N 6000 7944 9113 2056
NC1132	-.17867E+09	254805.5000	C H O N 6000 7941 9119 2059
NC1133	-.17860E+09	254934.2000	C H O N 6000 7938 9124 2062
NC1134	-.17853E+09	255063.1000	C H O N 6000 7935 9130 2065

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1135	-.17846E+09	255192.0000	C H O N 6000 7932 9136 2068
NC1136	-.17839E+09	255321.1000	C H O N 6000 7929 9142 2071
NC1137	-.17832E+09	255450.3000	C H O N 6000 7926 9147 2074
NC1138	-.17825E+09	255579.7000	C H O N 6000 7923 9153 2077
NC1139	-.17816E+09	255709.2000	C H O N 6000 7921 9159 2079
NC1140	-.17811E+09	255838.8000	C H O N 6000 7918 9165 2082
NC1141	-.17804E+09	255968.6000	C H O N 6000 7915 9170 2085
NC1142	-.17797E+09	256098.4000	C H O N 6000 7912 9176 2088
NC1143	-.17790E+09	256228.5000	C H O N 6000 7909 9182 2091
NC1144	-.17783E+09	256358.6000	C H O N 6000 7906 9188 2094
NC1145	-.17776E+09	256488.9000	C H O N 6000 7903 9193 2097
NC1146	-.17769E+09	256619.3000	C H O N 6000 7900 9199 2100
NC1147	-.17762E+09	256749.8000	C H O N 6000 7897 9205 2103
NC1148	-.17755E+09	256880.5000	C H O N 6000 7895 9211 2105
NC1149	-.17748E+09	257011.3000	C H O N 6000 7892 9217 2108
NC1150	-.17741E+09	257142.3000	C H O N 6000 7889 9222 2111
NC1151	-.17734E+09	257273.3000	C H O N 6000 7886 9228 2114

BLAKE NAME	HEAT GF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1152	-.17726E+09	257404.6000	C H O N 6000 7883 9234 2117
NC1153	-.17719E+09	257535.9000	C H O N 6000 7880 9240 2120
NC1154	-.17712E+09	257667.4000	C H O N 6000 7877 9246 2123
NC1155	-.17705E+09	257799.0000	C H O N 6000 7874 9252 2126
NC1156	-.17698E+09	257930.7000	C H O N 6000 7871 9258 2129
NC1157	-.17691E+09	258062.6000	C H O N 6000 7868 9263 2132
NC1158	-.17684E+09	258194.6000	C H O N 6000 7865 9269 2135
NC1159	-.17677E+09	258326.8000	C H O N 6000 7862 9275 2138
NC1160	-.17669E+09	258459.1000	C H O N 6000 7860 9281 2140
NC1161	-.17662E+09	258591.5000	C H O N 6000 7857 9287 2143
NC1162	-.17655E+09	258724.1000	C H O N 6000 7854 9293 2146
NC1163	-.17648E+09	258856.8000	C H O N 6000 7851 9299 2149
NC1164	-.17641E+09	258989.6000	C H O N 6000 7848 9305 2152
NC1165	-.17634E+09	259122.6000	C H O N 6000 7845 9310 2155
NC1166	-.17626E+09	259255.7000	C H O N 6000 7842 9316 2158
NC1167	-.17619E+09	259388.9000	C H O N 6000 7839 9322 2161
NC1168	-.17612E+09	259522.3000	C H O N 6000 7836 9328 2164

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1169	-.17605E+09	259655.8000	C H O N 6000 7833 9334 2167
NC1170	-.17598E+09	259789.4000	C H O N 6000 7830 9340 2170
NC1171	-.17590E+09	259923.2000	C H O N 6000 7827 9346 2173
NC1172	-.17583E+09	260057.2000	C H O N 6000 7824 9352 2176
NC1173	-.17576E+09	260191.2000	C H O N 6000 7821 9358 2179
NC1174	-.17569E+09	260325.4000	C H O N 6000 7818 9364 2182
NC1175	-.17561E+09	260459.8000	C H O N 6000 7815 9370 2185
NC1176	-.17554E+09	260594.3000	C H O N 6000 7812 9376 2188
NC1177	-.17547E+09	260728.9000	C H O N 6000 7809 9382 2191
NC1178	-.17540E+09	260863.6000	C H O N 6000 7806 9388 2194
NC1179	-.17532E+09	260998.5000	C H O N 6000 7803 9394 2197
NC1180	-.17525E+09	261133.6000	C H O N 6000 7800 9400 2200
NC1181	-.17518E+09	261268.8000	C H O N 6000 7797 9406 2203
NC1182	-.17510E+09	261404.1000	C H O N 6000 7794 9412 2206
NC1183	-.17503E+09	261539.5000	C H O N 6000 7791 9418 2209
NC1184	-.17496E+09	261675.1000	C H O N 6000 7788 9424 2212
NC1185	-.17488E+09	261810.9000	C H O N 6000 7785 9430 2215

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1186	-.17481E+09	261946.8000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7782 9436 2218
NC1187	-.17474E+09	262082.8000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7779 9442 2221
NC1188	-.17466E+09	262218.9000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7776 9448 2224
NC1189	-.17459E+09	262355.2000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7773 9454 2227
NC1190	-.17452E+09	262491.7000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7770 9460 2230
NC1191	-.17444E+09	262628.3000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7767 9466 2233
NC1192	-.17437E+09	262765.0000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7764 9472 2236
NC1193	-.17429E+09	262901.9000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7761 9478 2239
NC1194	-.17422E+09	263038.7000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7758 9485 2242
NC1195	-.17415E+09	263176.1000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7755 9491 2245
NC1196	-.17407E+09	263313.4000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7752 9497 2248
NC1197	-.17400E+09	263450.8000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7749 9503 2251
NC1198	-.17392E+09	263588.4000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7746 9509 2254
NC1199	-.17385E+09	263726.1000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7742 9515 2258
NC1200	-.17377E+09	263864.0000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7739 9521 2261
NC1201	-.17370E+09	264002.0000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7736 9527 2264
NC1202	-.17363E+09	264140.2000	C ⁴ H ⁰ O ⁰ N ⁰ 6000 7733 9533 2267

BLAKE NAME	HEAT OF FORMATION CAL./MOLE	MOL. WEIGHT	FORMULA
NC1203	-.17355E+09	264278.5000	C H O N 6000 7730 9540 2270
NC1204	-.17348E+09	264417.0000	C H O N 6000 7727 9546 2273
NC1205	-.17340E+09	264555.6000	C H O N 6000 7724 9552 2276
NC1206	-.17333E+09	264694.3000	C H O N 6000 7721 9558 2279
NC1207	-.17325E+09	264833.2000	C H O N 6000 7718 9564 2282
NC1208	-.17318E+09	264972.2000	C H O N 6000 7715 9570 2285
NC1209	-.17310E+09	265111.4000	C H O N 6000 7712 9577 2288
NC1210	-.17303E+09	265250.7000	C H O N 6000 7709 9583 2291
NC1211	-.17295E+09	265390.2000	C H O N 6000 7705 9589 2295
NC1212	-.17287E+09	265529.8000	C H O N 6000 7702 9595 2298
NC1213	-.17280E+09	265669.6000	C H O N 6000 7699 9601 2301
NC1214	-.17272E+09	265809.5000	C H O N 6000 7696 9608 2304
NC1215	-.17265E+09	265949.6000	C H O N 6000 7693 9614 2307
NC1216	-.17257E+09	266089.8000	C H O N 6000 7690 9620 2310
NC1217	-.17250E+09	266230.2000	C H O N 6000 7687 9626 2313
NC1218	-.17242E+09	266370.7000	C H O N 6000 7684 9633 2316
NC1219	-.17234E+09	266511.3000	C H O N 6000 7681 9639 2319

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1220	-.17227E+09	266652.1000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7677 9645 2323
NC1221	-.17219E+09	266793.1000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7674 9651 2326
NC1222	-.17212E+09	266934.2000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7671 9658 2329
NC1223	-.17204E+09	267075.4000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7668 9664 2332
NC1224	-.17196E+09	267216.9000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7665 9670 2335
NC1225	-.17189E+09	267358.4000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7662 9677 2338
NC1226	-.17181E+09	267500.1000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7659 9683 2341
NC1227	-.17173E+09	267642.0000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7655 9689 2345
NC1228	-.17166E+09	267784.0000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7652 9695 2348
NC1229	-.17158E+09	267926.1000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7649 9702 2351
NC1230	-.17150E+09	268068.4000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7646 9708 2354
NC1231	-.17143E+09	268210.9000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7643 9714 2357
NC1232	-.17135E+09	268353.5000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7640 9721 2360
NC1233	-.17127E+09	268496.2000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7636 9727 2364
NC1234	-.17119E+09	268639.2000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7633 9733 2367
NC1235	-.17112E+09	268782.2000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7630 9740 2370
NC1236	-.17104E+09	268925.4000	C ⁶ H ⁶ O ⁶ N ⁶ 6000 7627 9746 2373

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1237	-.17096E+09	269068.8000	C H O N 6000 7624 9753 2376
NC1238	-.17088E+09	269212.3000	C H O N 6000 7621 9759 2379
NC1239	-.17081E+09	269356.0000	C H O N 6000 7617 9765 2383
NC1240	-.17073E+09	269499.8000	C H O N 6000 7614 9772 2386
NC1241	-.17065E+09	269643.8000	C H O N 6000 7611 9778 2389
NC1242	-.17057E+09	269787.9000	C H O N 6000 7608 9785 2392
NC1243	-.17050E+09	269932.2000	C H O N 6000 7605 9791 2395
NC1244	-.17042E+09	270076.7000	C H O N 6000 7601 9797 2399
NC1245	-.17034E+09	270221.3000	C H O N 6000 7598 9804 2402
NC1246	-.17026E+09	270366.0000	C H O N 6000 7595 9810 2405
NC1247	-.17018E+09	270510.9000	C H O N 6000 7592 9817 2408
NC1248	-.17010E+09	270656.0000	C H O N 6000 7588 9823 2412
NC1249	-.17003E+09	270801.2000	C H O N 6000 7585 9830 2415
NC1250	-.16995E+09	270946.6000	C H O N 6000 7582 9836 2418
NC1251	-.16987E+09	271092.1000	C H O N 6000 7579 9842 2421
NC1252	-.16979E+09	271237.8000	C H O N 6000 7576 9849 2424
NC1253	-.16971E+09	271383.7000	C H O N 6000 7572 9855 2428

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1254	-.16963E+09	271529.7000	C ⁶⁰⁰⁰ H ⁷⁵⁶⁹ O ⁹⁸⁶² N ²⁴³¹
NC1255	-.16955E+09	271675.8000	C ⁶⁰⁰⁰ H ⁷⁵⁶⁶ O ⁹⁸⁶⁸ N ²⁴³⁴
NC1256	-.16947E+09	271822.1000	C ⁶⁰⁰⁰ H ⁷⁵⁶³ O ⁹⁸⁷⁵ N ²⁴³⁷
NC1257	-.16940E+09	271968.6000	C ⁶⁰⁰⁰ H ⁷⁵⁵⁹ O ⁹⁸⁸¹ N ²⁴⁴¹
NC1258	-.16932E+09	272115.2000	C ⁶⁰⁰⁰ H ⁷⁵⁵⁶ O ⁹⁸⁸⁸ N ²⁴⁴⁴
NC1259	-.16924E+09	272262.0000	C ⁶⁰⁰⁰ H ⁷⁵⁵³ O ⁹⁸⁹⁴ N ²⁴⁴⁷
NC1260	-.16916E+09	272409.0000	C ⁶⁰⁰⁰ H ⁷⁵⁴⁹ O ⁹⁹⁰¹ N ²⁴⁵¹
NC1261	-.16908E+09	272556.1000	C ⁶⁰⁰⁰ H ⁷⁵⁴⁶ O ⁹⁹⁰⁸ N ²⁴⁵⁴
NC1262	-.16900E+09	272703.4000	C ⁶⁰⁰⁰ H ⁷⁵⁴³ O ⁹⁹¹⁴ N ²⁴⁵⁷
NC1263	-.16892E+09	272850.8000	C ⁶⁰⁰⁰ H ⁷⁵⁴⁰ O ⁹⁹²¹ N ²⁴⁶⁰
NC1264	-.16884E+09	272998.4000	C ⁶⁰⁰⁰ H ⁷⁵³⁶ O ⁹⁹²⁷ N ²⁴⁶⁴
NC1265	-.16876E+09	273146.1000	C ⁶⁰⁰⁰ H ⁷⁵³³ O ⁹⁹³⁴ N ²⁴⁶⁷
NC1266	-.16868E+09	273294.0000	C ⁶⁰⁰⁰ H ⁷⁵³⁰ O ⁹⁹⁴⁰ N ²⁴⁷⁰
NC1267	-.16860E+09	273442.1000	C ⁶⁰⁰⁰ H ⁷⁵²⁷ O ⁹⁹⁴⁷ N ²⁴⁷³
NC1268	-.16852E+09	273590.3000	C ⁶⁰⁰⁰ H ⁷⁵²³ O ⁹⁹⁵⁴ N ²⁴⁷⁷
NC1269	-.16844E+09	273738.7000	C ⁶⁰⁰⁰ H ⁷⁵²⁰ O ⁹⁹⁶⁰ N ²⁴⁸⁰
NC1270	-.16836E+09	273887.2000	C ⁶⁰⁰⁰ H ⁷⁵¹⁷ O ⁹⁹⁶⁷ N ²⁴⁸³

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1271	-.16828E+09	274036.0000	C H O N 6000 7513 9973 2487
NC1272	-.16820E+09	274184.8000	C H O N 6000 7510 9980 2490
NC1273	-.16812E+09	274333.9000	C H O N 6000 7507 9987 2493
NC1274	-.16804E+09	274483.1000	C H O N 6000 7503 9993 2497
NC1275	-.16796E+09	274632.4000	C H O N 6000 7500 10000 2500
NC1276	-.16788E+09	274781.9000	C H O N 6000 7497 10006 2503
NC1277	-.16779E+09	274931.6000	C H O N 6000 7493 10013 2507
NC1278	-.16771E+09	275081.5000	C H O N 6000 7490 10020 2510
NC1279	-.16763E+09	275231.5000	C H O N 6000 7487 10026 2513
NC1280	-.16755E+09	275381.6000	C H O N 6000 7483 10033 2517
NC1281	-.16747E+09	275532.0000	C H O N 6000 7480 10040 2520
NC1282	-.16739E+09	275682.5000	C H O N 6000 7477 10047 2523
NC1283	-.16731E+09	275833.1000	C H O N 6000 7473 10053 2527
NC1284	-.16723E+09	275984.0000	C H O N 6000 7470 10060 2530
NC1285	-.16714E+09	276135.0000	C H O N 6000 7467 10067 2533
NC1286	-.16706E+09	276286.1000	C H O N 6000 7463 10073 2537
NC1287	-.16698E+09	276437.5000	C H O N 6000 7460 10080 2540

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1288	-.16690E+09	276588.9000	C H O N 6000 7457 10087 2543
NC1289	-.16682E+09	276740.6000	C H O N 6000 7453 10094 2547
NC1290	-.16674E+09	276892.4000	C H O N 6000 7450 10100 2550
NC1291	-.16665E+09	277044.4000	C H O N 6000 7446 10107 2554
NC1292	-.16657E+09	277196.6000	C H O N 6000 7443 10114 2557
NC1293	-.16649E+09	277348.9000	C H O N 6000 7440 10121 2560
NC1294	-.16641E+09	277501.4000	C H O N 6000 7436 10127 2564
NC1295	-.16632E+09	277654.1000	C H O N 6000 7433 10134 2567
NC1296	-.16624E+09	277806.9000	C H O N 6000 7430 10141 2570
NC1297	-.16616E+09	277959.9000	C H O N 6000 7426 10148 2574
NC1298	-.16608E+09	278113.0000	C H O N 6000 7423 10155 2577
NC1299	-.16599E+09	278266.4000	C H O N 6000 7419 10161 2581
NC1300	-.16591E+09	278419.9000	C H O N 6000 7416 10168 2584
NC1301	-.16583E+09	278573.6000	C H O N 6000 7412 10175 2588
NC1302	-.16574E+09	278727.4000	C H O N 6000 7409 10182 2591
NC1303	-.16566E+09	278881.4000	C H O N 6000 7406 10189 2594
NC1304	-.16558E+09	279035.6000	C H O N 6000 7402 10196 2598

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1305	-.16549E+09	279190.0000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7399 10202 2601
NC1306	-.16541E+09	279344.5000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7395 10209 2605
NC1307	-.16533E+09	279499.2000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7392 10216 2608
NC1308	-.16524E+09	279654.0000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7388 10223 2612
NC1309	-.16516E+09	279809.1000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7385 10230 2615
NC1310	-.16508E+09	279964.3000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7382 10237 2618
NC1311	-.16499E+09	280119.7000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7378 10244 2622
NC1312	-.16491E+09	280275.2000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7375 10251 2625
NC1313	-.16482E+09	280431.0000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7371 10258 2629
NC1314	-.16474E+09	280586.9000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7368 10264 2632
NC1315	-.16465E+09	280742.9000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7364 10271 2636
NC1316	-.16457E+09	280899.2000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7361 10278 2639
NC1317	-.16449E+09	281055.6000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7357 10285 2643
NC1318	-.16440E+09	281212.2000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7354 10292 2646
NC1319	-.16432E+09	281369.0000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7350 10299 2650
NC1320	-.16423E+09	281525.9000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7347 10306 2653
NC1321	-.16415E+09	281683.0000	C ⁴ H ⁰ D ⁰ N ⁰ 6000 7343 10313 2657

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1322	-.16406E+09	281840.3000	C ⁶⁰⁰⁰ H ⁷³⁴⁰ O ¹⁰³²⁰ N ²⁶⁶⁰
NC1323	-.16398E+09	281997.8000	C ⁶⁰⁰⁰ H ⁷³³⁶ O ¹⁰³²⁷ N ²⁶⁶⁴
NC1324	-.16389E+09	282155.5000	C ⁶⁰⁰⁰ H ⁷³³³ O ¹⁰³³⁴ N ²⁶⁶⁷
NC1325	-.16381E+09	282313.3000	C ⁶⁰⁰⁰ H ⁷³²⁹ O ¹⁰³⁴¹ N ²⁶⁷¹
NC1326	-.16372E+09	282471.3000	C ⁶⁰⁰⁰ H ⁷³²⁶ O ¹⁰³⁴⁸ N ²⁶⁷⁴
NC1327	-.16364E+09	282629.5000	C ⁶⁰⁰⁰ H ⁷³²² O ¹⁰³⁵⁵ N ²⁶⁷⁸
NC1328	-.16355E+09	282787.8000	C ⁶⁰⁰⁰ H ⁷³¹⁹ O ¹⁰³⁶² N ²⁶⁸¹
NC1329	-.16346E+09	282946.4000	C ⁶⁰⁰⁰ H ⁷³¹⁵ O ¹⁰³⁶⁹ N ²⁶⁸⁵
NC1330	-.16338E+09	283105.1000	C ⁶⁰⁰⁰ H ⁷³¹² O ¹⁰³⁷⁶ N ²⁶⁸⁸
NC1331	-.16329E+09	283264.0000	C ⁶⁰⁰⁰ H ⁷³⁰⁸ O ¹⁰³⁸³ N ²⁶⁹²
NC1332	-.16321E+09	283423.0000	C ⁶⁰⁰⁰ H ⁷³⁰⁵ O ¹⁰³⁹¹ N ²⁶⁹⁵
NC1333	-.16312E+09	283582.3000	C ⁶⁰⁰⁰ H ⁷³⁰¹ O ¹⁰³⁹⁸ N ²⁶⁹⁹
NC1334	-.16303E+09	283741.7000	C ⁶⁰⁰⁰ H ⁷²⁹⁸ O ¹⁰⁴⁰⁵ N ²⁷⁰²
NC1335	-.16295E+09	283901.3000	C ⁶⁰⁰⁰ H ⁷²⁹⁴ O ¹⁰⁴¹² N ²⁷⁰⁶
NC1336	-.16286E+09	284061.1000	C ⁶⁰⁰⁰ H ⁷²⁹¹ O ¹⁰⁴¹⁹ N ²⁷⁰⁹
NC1337	-.16278E+09	284221.1000	C ⁶⁰⁰⁰ H ⁷²⁸⁷ O ¹⁰⁴²⁶ N ²⁷¹³
NC1338	-.16269E+09	284381.2000	C ⁶⁰⁰⁰ H ⁷²⁸³ O ¹⁰⁴³³ N ²⁷¹⁷

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1339	-.16260E+09	284541.5000	C H O N 6030 7280 10440 2720
NC1340	-.16252E+09	284702.0000	C H O N 6000 7276 10447 2724
NC1341	-.16243E+09	284862.7000	C H O N 6000 7273 10455 2727
NC1342	-.16234E+09	285023.6000	C H O N 6000 7269 10462 2731
NC1343	-.16225E+09	285184.7000	C H O N 6000 7266 10469 2734
NC1344	-.16217E+09	285345.9000	C H O N 6000 7262 10476 2738
NC1345	-.16208E+09	285507.3000	C H O N 6000 7258 10483 2742
NC1346	-.16199E+09	285668.9000	C H O N 6000 7255 10490 2745
NC1347	-.16191E+09	285830.7000	C H O N 6000 7251 10498 2749
NC1348	-.16182E+09	285992.6000	C H O N 6000 7246 10505 2752
NC1349	-.16173E+09	286154.8000	C H O N 6000 7244 10512 2756
NC1350	-.16164E+09	286317.1000	C H O N 6000 7240 10519 2760
NC1351	-.16156E+09	286479.6000	C H O N 6000 7237 10526 2763
NC1352	-.16147E+09	286642.3000	C H O N 6000 7233 10534 2767
NC1353	-.16138E+09	286805.2000	C H O N 6000 7230 10541 2770
NC1354	-.16129E+09	286968.3000	C H O N 6000 7226 10548 2774
NC1355	-.16120E+09	287131.6000	C H O N 6000 7222 10555 2778

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1356	-.16111E+09	287295.0000	C H O N 6000 7219 10563 2781
NC1357	-.16103E+09	287458.6000	C H O N 6000 7215 10570 2785
NC1358	-.16094E+09	287622.5000	C H O N 6000 7211 10577 2789
NC1359	-.16085E+09	287786.5000	C H O N 6000 7208 10584 2792
NC1360	-.16076E+09	287950.6000	C H O N 6000 7204 10592 2796
NC1361	-.16067E+09	288115.0000	C H O N 6000 7200 10599 2800
NC1362	-.16058E+09	288279.6000	C H O N 6000 7197 10606 2803
NC1363	-.16049E+09	288444.3000	C H O N 6000 7193 10614 2807
NC1364	-.16040E+09	288609.3000	C H O N 6000 7189 10621 2811
NC1365	-.16032E+09	288774.4000	C H O N 6000 7186 10628 2814
NC1366	-.16023E+09	288939.7000	C H O N 6000 7182 10636 2818
NC1367	-.16014E+09	289105.2000	C H O N 6000 7178 10643 2822
NC1368	-.16005E+09	289270.9000	C H O N 6000 7175 10650 2825
NC1369	-.15996E+09	289436.8000	C H O N 6000 7171 10658 2829
NC1370	-.15987E+09	289602.9000	C H O N 6000 7167 10665 2833
NC1371	-.15978E+09	289769.2000	C H O N 6000 7164 10673 2836
NC1372	-.15969E+09	289935.6000	C H O N 6000 7160 10680 2840

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1373	-.15960E+09	290102.3000	C ⁶⁰⁰⁰ H ⁷¹⁵⁶ O ¹⁰⁶⁸⁷ N ²⁸⁴⁴
NC1374	-.15951E+09	290269.1000	C ⁶⁰⁰⁰ H ⁷¹⁵³ O ¹⁰⁶⁹⁵ N ²⁸⁴⁷
NC1375	-.15942E+09	290436.2000	C ⁶⁰⁰⁰ H ⁷¹⁴⁹ O ¹⁰⁷⁰² N ²⁸⁵¹
NC1376	-.15933E+09	290603.4000	C ⁶⁰⁰⁰ H ⁷¹⁴⁵ O ¹⁰⁷¹⁰ N ²⁸⁵⁵
NC1377	-.15924E+09	290770.8000	C ⁶⁰⁰⁰ H ⁷¹⁴¹ O ¹⁰⁷¹⁷ N ²⁸⁵⁹
NC1378	-.15915E+09	290938.4000	C ⁶⁰⁰⁰ H ⁷¹³⁸ O ¹⁰⁷²⁵ N ²⁸⁶²
NC1379	-.15906E+09	291106.2000	C ⁶⁰⁰⁰ H ⁷¹³⁴ O ¹⁰⁷³² N ²⁸⁶⁶
NC1380	-.15896E+09	291274.2000	C ⁶⁰⁰⁰ H ⁷¹³⁰ O ¹⁰⁷⁴⁰ N ²⁸⁷⁶
NC1381	-.15887E+09	291442.4000	C ⁶⁰⁰⁰ H ⁷¹²⁷ O ¹⁰⁷⁴⁷ N ²⁸⁷³
NC1382	-.15878E+09	291610.8000	C ⁶⁰⁰⁰ H ⁷¹²³ O ¹⁰⁷⁵⁴ N ²⁸⁷⁷
NC1383	-.15869E+09	291779.4000	C ⁶⁰⁰⁰ H ⁷¹¹⁹ O ¹⁰⁷⁶² N ²⁸⁸¹
NC1384	-.15860E+09	291948.2000	C ⁶⁰⁰⁰ H ⁷¹¹⁵ O ¹⁰⁷⁶⁹ N ²⁸⁸⁵
NC1385	-.15851E+09	292117.2000	C ⁶⁰⁰⁰ H ⁷¹¹² O ¹⁰⁷⁷⁷ N ²⁸⁸⁸
NC1386	-.15842E+09	292286.3000	C ⁶⁰⁰⁰ H ⁷¹⁰⁸ O ¹⁰⁷⁸⁵ N ²⁸⁹²
NC1387	-.15833E+09	292455.7000	C ⁶⁰⁰⁰ H ⁷¹⁰⁴ O ¹⁰⁷⁹² N ²⁸⁹⁶
NC1388	-.15823E+09	292625.3000	C ⁶⁰⁰⁰ H ⁷¹⁰⁰ O ¹⁰⁸⁰⁰ N ²⁹⁰⁰
NC1389	-.15814E+09	292795.0000	C ⁶⁰⁰⁰ H ⁷⁰⁹⁶ O ¹⁰⁸⁰⁷ N ²⁹⁰⁴

BLAKE NAME	HEAT OF FORMATION CAL/MOLE	MOL. WEIGHT	FORMULA
NC1390	-.15805E+09	292965.0000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁹³ N ¹⁰⁸¹⁵ 2907
NC1391	-.15796E+09	293135.1000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁸⁹ N ¹⁰⁸²² 2911
NC1392	-.15787E+09	293305.5000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁸⁵ N ¹⁰⁸³⁰ 2915
NC1393	-.15778E+09	293476.0000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁸¹ N ¹⁰⁸³⁷ 2919
NC1394	-.15768E+09	293646.8000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁷⁸ N ¹⁰⁸⁴⁵ 2922
NC1395	-.15759E+09	293817.7000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁷⁴ N ¹⁰⁸⁵³ 2926
NC1396	-.15750E+09	293988.9000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁷⁰ N ¹⁰⁸⁶⁰ 2930
NC1397	-.15741E+09	294160.2000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁶⁶ N ¹⁰⁸⁶⁸ 2934
NC1398	-.15731E+09	294331.8000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁶² N ¹⁰⁸⁷⁵ 2938
NC1399	-.15722E+09	294503.5000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁵⁸ N ¹⁰⁸⁸³ 2942
NC1400	-.15713E+09	294675.5000	C ⁶ H ⁰⁰⁰⁰ O ⁷⁰⁵⁵ N ¹⁰⁸⁹¹ 2945

APPENDIX C
OUTPUT FROM TEST CASES

** PROGRAM BLAKE, VERSION 205.0 **
 TYGER! TYGER! BURNING BRIGHT/ IN THE FORESTS OF THE NIGHT,
 WHAT IMMORTAL HAND OR EYE/ DARE FRAME THY FEARFUL SYMMETRY?
 ---WILLIAM BLAKE (1757-1827)

20 JUL, 1981

COMMENT: TEST CASES FOR 'BLAKE'

**** UNITS, ENG

**NOTE: THE USE OF ENGLISH UNITS IS TO BE DEPRECATED. SI UNITS ARE COMING. YOU WON'T LEARN THEM IF YOU DON'T USE THEM!
 **

**** DATE, TEST DAY, 1981

**** FORMULA, KCRY, -793E3, K,3,AL,1,F,6

**** TIT, BLAKE TEST CASE NO. 1: M1A1

**** PRL, CON, 2

**** COM, NC1260, 83.173, DNT, 9.843, DBP, 4.429, DPA, .984, ETOH, .98, H2O,
 **

* * USING THE BINARY LIBRARY CREATED ON 19 JAN, 1981 * *

BLAKE TEST CASE NO. 1: MIAL

THE COMPOSITION IS

NAME	PCT Wt	PCT MOLE	DEL H-LAL/M	FORMULA
NC1260	98.986	83.667	-1.6916E+08	C 6000 7547 9901 2451
UNT	.008	9.902	-1.7160E+04	C 7 4 6 0 4 2
DBP	.005	4.455	-2.0140E+03	C 16 4 22 0 4
DPA	.001	.990	3.1070E+04	C 12 4 1 11
ETOH	.000	.900	-6.6420E+04	C 2 4 6 1

THE HEAT OF FORMATION IS -620.94 CAL/GRAM = -1.4154E+08 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	23.169
H	29.148
O	38.222
N	9.462

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 2

BLAKE TEST CASE NO. 1: 41A1

THERE ARE 21 GASEOUS CONSTITUENTS SELECTED

NAME	BKW	L-J	EPS/K	L-J	SIGMA	A1	A2	A3	A4	A5	A6	A7	A8	A9
1. CC	390.0	91.7	3.69C	5.83775	-0.40270	0.6491	-0.0373	-2.14066	0.71717	-0.08241	-3.1130.5	53.1746		
2. H2I	250.0	542.5	2.790	7.60069	0.39388	-0.10260	0.0607	-4.86936	2.30899	-0.37689	-62860.1	47.10C8		
3. CO2	600.0	195.2	3.941	9.06744	-0.0694	0.06138	-0.00273	-2.70529	0.56199	-0.04428	-102647.7	60.2574		
4. N2	380.0	71.4	3.798	5.90618	-0.39603	0.5863	-0.0307	-2.41322	0.89566	-0.11540	-4589.1	-1.2456		
5. H2	190.0	59.7	2.827	4.48064	0.19824	-0.06851	-0.0003	-1.97442	1.15151	-0.21216	-2116.7	30.2744		
6. CH	386.0	116.7	3.492	5.77838	-0.43892	0.08202	-0.00561	-1.79245	0.50895	-0.04564	16765.3	57.0969		
7. NH3	476.0	558.3	2.900	13.60829	-0.93312	0.18185	-0.00958	-9.06058	3.51672	-0.50840	-22985.7	45.5074		
8. HCN	359.0	344.7	3.339	9.48792	-0.37343	0.4424	-0.00222	-4.59416	1.73907	-0.25679	24383.5	53.6459		
9. CH4	528.0	148.6	3.758	20.35251	-1.95871	0.26284	-0.01397	-14.43243	5.11197	-0.67906	-38010.8	38.5449		
10. C2H4	372.0	224.7	4.163	22.63477	-1.64131	0.2002	-0.00937	-13.78191	4.49325	-0.59268	-10548.7	51.3360		
11. C2H2	0.0	100.0	3.900	12.54085	-1.6675	0.02155	-0.00023	-5.90900	2.01409	-0.26643	43014.0	54.7220		
12. O2	350.0	106.7	3.467	2.20306	1.12042	-0.18485	0.1276	2.02364	-1.20737	0.22334	-2085.5	59.2300		
13. C2N2	0.0	100.0	3.500	13.82927	-1.13108	0.19089	-0.01253	-5.06809	1.56648	-0.19796	61813.4	76.4037		
14. C	159.6	100.0	3.500	2.48078	-0.11622	0.06890	-0.00721	-1.5769	-0.10342	0.01993	169338.0	44.1829		
15. OH	226.0	100.0	3.500	4.22400	0.47240	-0.11211	0.0042	-1.70189	0.97134	-0.16944	7437.0	49.0478		
16. CH3	525.0	100.0	3.500	13.82287	-0.74765	0.05695	-0.00032	-0.14376	3.65133	-0.54025	23004.1	46.4265		
17. H	13.4	100.0	3.500	2.49993	0.00000	-0.00000	0.00000	0.00000	-0.00000	0.00000	50621.8	33.4041		
18. D	212.8	100.0	3.500	2.97972	-0.25641	0.05953	-0.00389	-0.43119	1.9753	-0.02943	57760.7	44.3789		
19. CHD	700.0	100.0	3.500	10.04357	-1.09647	0.20869	-0.01480	-4.57561	1.36619	-0.14753	955.9	59.4686		
20. CH2	525.0	100.0	3.500	11.42150	-1.32276	0.21610	-0.01403	-7.38097	3.01187	-0.44496	83047.1	47.9048		
21. CN	0.0	100.0	3.500	2.71179	0.54169	0.09568	-0.02040	1.50282	-1.01851	0.20537	101465.0	56.3631		

THE FLOOR IS AT 12

THERE ARE 1 CONDENSED CONSTITUENTS SELECTED:

NAME		THERMO CONSTS (LIQUID FIRST, THEN SOLID)		FOLLOWED BY CONDENSED EON OF STATE		CONSTS (LIQUID FIRST, THEN SOLID)				
(FRMS IN LIB	PRT)	B1/C1	82/C2	83/C3	84/C4	85/C5	86/C6	87/C7	88/C8	89/C9
1.	C(S)	0.	0.	0.	0.	0.	0.	0.	0.	0.
		4.01949E+00	-4.08033E-01	8.28917E-02	-4.97439E-03	-1.05594E+00	-8.19033E-02	4.58611E-02	-4.91945E+03	4.45424E+C0
		0.	0.	0.	0.	0.	0.	0.	0.	0.
		4.99259E+00	3.96280E-05	1.19136E-09	-6.37753E-06	1.19250E-10	-3.75578E-15	3.58287E-12	-1.00976E-16	4.

***** GUN, 0.05, 0.08

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 3

BLAKE TEST CASE NO. 1: MIAL

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	1)
CO GAS	1.71111E+01
H2O GAS	9.30617E+00
CO2 GAS	4.91493E+00
N2 GAS	4.49237E+00
H2 GAS	4.45102E+00
NO GAS	9.44710E-03
NH3 GAS	1.86292E-03
HCN GAS	8.92129E-04
O2 GAS	1.14099E-03
CH4 GAS	1.31855E-03
C2H2 GAS	3.12425E-07
C2H4 GAS	2.26810E-09
C2H6 GAS	3.79403E-09
C GAS	6.74342E-09
OH GAS	8.06297E-02
CH3 GAS	7.38030E-06
H GAS	1.11572E-01
O GAS	1.25760E-03
CHD GAS	1.94112E-03
CH2 GAS	3.94578E-07
CN GAS	3.23344E-06

C(S) SOLID 0.

TOTAL GAS (MOLES/KG) 40.4843

PROGRAM BLAKE, VERSION 203.0

TE, TEST DAY, 1981 PAGE 4

BLAKE TEST CASE NO. 1: M1A1

SUMMARY OF PROPELLANT THERMO PROPERTIES

RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT	CO-VOL CC/G	FROZEN GAMMA	CP(FR) J/MOL-K	B(T) CC	C(T) CM**6	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1) .0500	3075.	54.68	2034.9	24.701	1.074	1.2301	44.66	26.87	570.	20.000	9.55	-1504.4	-2598.0	1.2835	1.0567
RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT	CO-VOL CU IN	FROZEN GAMMA	CP(FR) CAL/M-K	B(T) CU IN	C(T) IN**6	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1) .0500	3075.	7931.	346242.	24.701	29.72	1.2301	10.67	1.640	2.12	552.598	2.28	-359.6	-620.9	1.2835	1.0567

DESTROY

REJ, O2, C(S)

REJ, C2N, C2H, C2, CH2O, NO2, H2S, S2O, K\$, KOH\$, K2O,

REJ, K2O2, K2O, HNO3, C, CH, K2, N,

REJ, KCO\$, KSO\$, K2O\$, NA2\$

REJ, C2H4, C2N2, C2H2, CH2

REJ, ALN, COF2, F2, ALF3, ALD, ALF2, A-2D, AL\$, ALH

RET

TIT, BLAKE TEST CASE NO. 2: M15

COM, NC1315, 19.94, NG, 18.943, NQ, 54.536, KCRV, .259, EC, 5.982, ETOH,

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 5

BLAKE TEST CASE NO. 2: M15

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1315	99.792	20.000	-1.6465E+08	C 6000 H 7364 O 10271 N 2636
N3	.077	19.000	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	.101	54.700	-2.2100E+04	C 1 H 4 O 2 N 4
KCRY	.001	.300	-7.4500E+05	K 3 AL 1 F 6
EC	.029	6.000	-2.5100E+04	C 17 H 20 O 1 N 2

THE HEAT OF FORMATION IS -585.84 CAL/GRAM = -3.2963E+07 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	22.826
H	28.048
O	39.060
N	10.065
K	.000
AL	.000
F	.000

**** GUN. 0.95, 0.05, 0.00

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 6

BLAKE TEST CASE NO. 2: M15

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	CONCENTRATION	PHASE
CO	1.58054E+01	GAS
H2O	9.43410E+00	GAS
CO2	5.55867E+00	GAS
N2	4.69609E+00	GAS
42	3.32496E+00	GAS
NO	2.76125E-02	GAS
N13	1.26179E-03	GAS
HCH	6.28150E-04	GAS
4F	3.19637E-04	GAS
KOH	1.33717E-04	GAS
ALH02	4.68136E-05	GAS
CH4	3.99628E-04	GAS
ALOH	5.63753E-05	GAS
AL	1.64122E-07	GAS
ALOF	2.50582E-08	GAS
ALF	7.42333E-09	GAS
AL02	0.	GAS
K	2.54423E-05	GAS
OH	1.79932E-01	GAS
KO	7.53675E-07	GAS
CH3	4.11668E-06	GAS
H	1.68504E-01	GAS
D	5.23548E-03	GAS
CH0	2.39321E-03	GAS
CM	5.09479E-06	GAS
AL02	6.96920E-07	GAS
F	1.50603E-07	GAS
K2CO3\$	0.	SOLID
K2CO3\$	0.	LIQUID
AL2O3\$	0.	SOLID
AL2O3\$	0.	LIQUID
TOTAL GAS (MOLES/KG)	39.3954	

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 7

BLAKE TEST CASE NO. 2: M15

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

RHO/L	TEMP	PRESSURE	IMPETUS	MOL WT	CO-VOL	FROZEN	CP(ER)	B(T)	C(T)	GAS VOL	S	H	J/G	E	ADEXP	PHI
G/CC	K	MPA	J/G	GAS	CC/G	GAMMA	J/MOL-K	CC	CH**6	CC/G	J/G-K	J/G	J/G	J/G		
1) .0500	3278.	56.70	1073.8	25.384	1.060	1.2243	45.56	27.27	583.	20.000	9.50	-1317.2	-2451.2		1.2690	1.0560

RHO/L	TEMP	PRESSURE	IMPETUS	MOL WT	CO-VOL	FROZEN	CP(ER)	B(T)	C(T)	GAS VOL	S	H	J/G	E	ADEXP	PHI
G/CC	K	PSI	FT-LB/L8	GAS	CU IN	GAMMA	CAL/M-K	CU IN	IN**6	CU IN/L8	GI885	CAL/MOL	CAL/MOL			
1) .0500	3278.	8223.	359757.	25.384	-9.32	1.2243	10.89	1.664	2.17	553.598	2.27	-314.8	-585.8		1.2690	1.0560

***** TIT, BLAKE TEST CASE NO. 3: T29

***** DESTROY

***** REJ, C2H, C2N, C2, N, C, CH, CH2, C2H2, C2H4, CH2O, CHO

***** REJ, HNO, HNO3

***** RET

***** COM, NC1315, 45.954, NG, 21.478, NL, 30.664, EC, 1.5, ETOM, .3, C, .1

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 8

BLAKE TEST CASE NO. 3: T29

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1315	45.454	.040	-1.6465E+08	C 6000 H 7364 O 10271 N 2636
NG	21.478	23.076	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	30.669	71.901	-2.2100E+04	C 1 H 4 O 2 N 4
EC	1.500	1.364	-2.5100E+04	C 17 H 20 O 1 P 2
ETOM	.300	1.569	-6.6420E+04	C 2 H 6 O 1
C	.100	2.031	0.	C 1

THE HEAT OF FORMATION IS -424.16 CAL/GRAM = -1.0349E+05 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C 17.245
H 30.933
O 32.229
N 19.593

***** GUN, 0.65, 0.05, 0.08

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 9

BLAKE TEST CASE NO. 3: T29

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	1)
CO	1.27882E+01
H2O	1.04188E+01
N2	9.51188E+00
H2	4.47029E+00
CO2	3.98089E+00
NO	2.53855E-02
NH3	2.63007E-03
HCl	9.13350E-04
O2	2.95766E-03
CH4	6.94622E-06
C2H2	4.27525E-09
OH	1.37304E-01
CH3	5.26720E-06
H	1.55579E-01
O	2.93556E-03
CN	5.08648E-06

110

C(S) SOLID Q.

TOTAL GAS (MOLES/KG) 41.4978

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 10

BLAKE TEST CASE NO. 3: T29

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

RHD/L	TEMP	PRESSURE	IMPETUS	MOL WT	CO-VOL	FROZEN	CP(FR)	B(T)	C(T)	GAS VOL	S	H	E	ADEXP	PHI
G/CC	K	MPA	J/G	GAS	CC/G	GAMMA	J/MOL-K	CC	CH**6	CC/G	J/G-K	J/G	J/G		
1) .0500	3200.	58.38	1104.0	24.098	1.090	1.2305	44.54	26.61	565.	20.000	9.76	-607.1	-1774.7	1.2791	1.0576
RHD/L	TEMP	PRESSURE	IMPETUS	MOL WT	CO-VOL	FROZEN	CP(FR)	B(T)	C(T)	GAS VOL	S	H	E	ADEXP	PHI
G/CC	K	PSI	FT-LB/LB	GAS	CU IN	GAMMA	CAL/M-K	CU IN	IN**6	CU IN/LB	GIBBS	CAL/MOL	CAL/MOL		
1) .0500	3200.	8467.	369341.	24.098	30.17	1.2305	10.65	1.624	2.11	553.598	2.34	-145.1	-424.2	1.2791	1.0576

***** TIT, BLAKE TEST CASE NO. 4: M9

***** PRL, FII, 0

***** COM, NC1325, 58.33, NG, 40.4, EC, .76, ETOH, .51

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 11

BLAKE TEST CASE NO. 4: M9

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1325	58.330	.108	-1.6381E+08	C 6000 H 7329 O 10341 N 2671
NG	40.400	92.652	-8.8600E+04	C 3 H 5 O 9 N 3
EC	.760	1.475	-2.5100E+04	C 17 H 20 O 1 N 2
ETOH	.510	5.765	-6.6420E+04	C 2 H 6 O 1

THE HEAT OF FORMATION IS -504.14 CAL/GRAM = -2.6256E+C5 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	20.011
H	27.426
O	40.719
N	11.844

***** GUN, 0.05, 0.05, 0.08

** PROGRAM BLAKE, VERSION 299.0 **

TE, TEST DAY, 1981 PAGE 12

BLAKE TEST CASE NO. 4: M9

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	CONCENTRATION
CO GAS	1.10652E+01
H2O GAS	1.01799E+01
CO2 GAS	7.37135E+00
N2 GAS	5.33760E+00
H2 GAS	1.66034E+00
NO GAS	2.36506E-01
O2 GAS	1.84972E-01
NH3 GAS	4.79742E-04
HCN GAS	1.93726E-04
CH4 GAS	2.03112E-07
C2H2 GAS	0.
OH GAS	8.42284E-01
CH3 GAS	6.74844E-07
H GAS	3.04931E-01
O GAS	8.01217E-02
CN GAS	7.00324E-06
C(S) SOLID	0.

TOTAL GAS (MOLES/KG) 37.4835

** PROGRAM BLAKE, VERSION 203.0 **

TE, TEST DAY, 1981 PAGE 13

BLAKE TEST CASE NO. 4: M9

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT GAS	CO-VOL CC/G	FROZEN GAMFA	CP(FR) J/MOL-K	B(T) CC	C(T) CH**6	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1) .0500	3700.	60.76	1153.2	26.678	1.021	1.2106	47.95	27.62	602.	20.000	9.50	-894.2	-2109.3	1.2222	1.0538
RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT GAS	CO-VOL CU IN	FROZEN GAMMA	CP(FR) CAL/M-K	B(T) CU IN	C(T) IN**6	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1) .0500	3700.	8812.	385796.	26.678	26.25	1.2106	11.46	1.685	2.24	953.598	2.27	-213.7	-504.1	1.2222	1.0538

***** TIT, BLAKE TEST CASE NO. 5: M10

***** CON, NC1315, 79.600, NG, 9.95, DBP, 8.955, DPA, .995, ETOH, .5,

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 14

BLAKE TEST CASE NO. 5: M18

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1315	79.600	.305	-1.6465E+08	C 6000 H 7364 O 10271 N 2436
NG	9.950	47.112	-8.8600E+04	C 3 H 5 O 9 N 3
DBP	8.955	34.592	-2.0140E+05	C 16 H 22 O 4
DPA	.995	6.322	3.1070E+04	C 12 H 11
ETOH	.500	11.670	-6.6420E+04	C 2 H 6 O 1

THE HEAT OF FORMATION IS -575.93 CAL/GRAM = -6.1915E+05 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C 24.606
H 31.715
O 34.756
N 8.923

***** GUN, 0.05, 0.05, 0.08

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 15

BLAKE TEST CASE NO. 5: M18

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6-12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	CONCENTRATION
CO	2.15167E+01
H2	8.58674E+00
H2O	7.18433E+00
N2	4.41821E+00
CO2	2.87634E+00
NH3	6.04167E-03
HCl	3.23192E-03
NO	5.12349E-04
CH4	5.13243E-06
C2H2	1.03069E-08
OH	6.13055E-03
CH3	4.66009E-05
H	3.31304E-02
D	1.64017E-05
CH	1.13918E-06
C(S)	SOLID
	0.
TOTAL GAS (MOLES/KG)	44.5530

BLAKE TEST CASE NO. 5: M18

** SUMMARY OF PROPELLANT THERMO PROPERTIES **

RHO/L G/CC	TEMP K	TEMP C	PRESSURE MPA	IMPETUS J/G	MOL WT GAS	CO-VOL CC/G	FROZEN GAMMA	CP(FR) J/MOL-K	B(T) CC	C(T) CC	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1) .0900	2606.		51.23	965.4	22.445	1.150	1.2538	41.28	26.38	543.	20.000	9.75	-1384.6	-2409.3	1.3236	1.0614
RHO/L G/CC	TEMP K	TEMP C	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT GAS	CO-VOL CU IN	FROZEN GAMMA	CP(FR) CAL/M-K	B(T) CU IN	C(T) CU IN	GAS VOL CU IN/LB	S GTBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1) .0900	2606.		7431.	325960.	22.445	32.05	1.2538	9.87	1.610	2.02	553.598	2.33	-330.9	-575.8	1.3236	1.0614

**** FOR, S, 0.0, S, 8000

**** FOR, WATER, -68.315E6, H, 2000, D, 1000

**** FOR, NZ, 0.0, N, 1000

**** FOR, KN03, -117.76E6, K, 1000, N, 1000, D, 3000

**** FOR, ASH, 0.0, K, 1000

**** FOR, SUSQUE, 0.000, C, 13208, H, 5734, D, 1000

**** DES

**** ORD, CC, K, CO2, N2, H2O, SO

**** ORC, K2SO4\$

**** REJ, C, CH, CH2, CH3, C2H6, C3H8, C2H2

**** REJ, S2O, C2, C2N, C2H, C(S)

**** REJ, K2SO4, KOH\$

**** RET

**** PRL, CON, O, PAG, O

**** TIT, BLAKE TEST CASE NO. 6: DUPONT 3014

***** CM2,KN03,73.878,S,9.985,SUSQUE,15.296,NZ,.049,ASH,.141

***** ,WATER,.65

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 17

BLAKE TEST CASE NO. 6: DUPONT 3814

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
KND3	73.879	81.407	-1.1776E+08	K 1000 N 1000 O 3000
S	9.985	4.337	0.	S 8000
SUSQUE	15.296	9.445	0.	C 13208 H 5734 O 1000
NZ	.049	.390	0.	N 1000
ASH	.141	.402	0.	K 1300
WATER	.650	4.020	-6.8315E+07	H 2000 O 1000

THE HEAT OF FORMATION IS -885.15 CAL/GRAM = -9.8611E+07 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

K 12.724
N 12.722
O 40.080
S 5.397
C 19.403
H 9.674

***** GUN, .0373, 10, 0

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT	CO-VOL CC/G	FROZEN GAS	CP(FR) J/MOL-K	B(T) CC	C(T) CC	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1) .0373	2189.	10.78	279.6	32.337	.876	1.2366	43.59	30.95	695.	26.408	5.97	-3414.5	-3703.5	1.1325	1.0183
RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT	CO-VOL CU IN	FROZEN GAS	CP(FR) CAL/M-K	B(T) CU IN	C(T) CU IN	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1) .0373	2189.	1564.	93531.	32.337	24.25	1.2366	10.42	1.889	2.59	730.972	1.43	-816.1	-885.2	1.1325	1.0183

***** SAV, ONE

SAVING LAST COMPUTED POINT NAMED ONE

***** PRL,CON,O,PAG,O

***** TIT,BLAKE TEST CASE NO. 7: DUPONT 7625

***** CM2,KN03,73.592,S,10.627,SUSQUE,14.451,NZ,.046,ASH,

***** .133, WATER, 1.151

** PROGRAM BLAKE, VERSION 205.0 **

TE, 1553 DAY- 1991 PAGE 18

BLAKE TEST CASE NO. 7: DUP:NT 7625

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/H	FORMULA
KN03	73.592	79.119	-1.1775E+08	K 1000 O 3000
S	10.627	4.504	0.	S 8000
SUSQUE	14.451	8.706	0.	C 4 H 4 O 1000
NZ	.046	.357	0.	N 1006
ASH	.133	.370	0.	K 1000
WATER	1.151	6.945	-6.8315E+07	H 2000 O 1000

THE HEAT OF FORMATION IS -980.61 CAL/GRAM = -9.7913E+07 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

N	12.632
O	12.680
S	40.365
C	5.748
H	18.346
	10.180

***** REC, ONE

RECALLING POINT ONE.

***** GUN, .0373, 1G, 0

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT GAS	CO-VOL. CC/G	FROZEN GAMMA	CP(FR) J/MOL-K	B(T) CC	C(T) CM**6	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1) .0373	2195.	10.63	275.0	33.004	.858	1.2312	44.44	30.49	690.	26.409	5.93	-3484.0	-3769.0	1.1294	1.0176
RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LB	MOL WT GAS	CO-VOL CU IN	FROZEN GAMMA	CP(FR) CAL/M-K	B(T) CU IN	C(T) IN**5	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1) .0373	2195.	1542.	92309.	33.004	23.75	1.2312	10.62	4.860	2.57	731.011	1.42	-832.7	-960.8	1.1294	1.0176

***** CMT ADIABATIC EXPANSION FOLLOWING CONSTANT VOLUME EXPLOSION

COMMENT: ADIABATIC EXPANSION FOLLOWING CONSTANT VOLUME EXPLOSION

***** PRL,CON,0

***** DES

***** TIT,8LAKE TEST CASE NO. 8: A TYPICAL DOUBLE BASE COMPOSITION

***** CON, NC1260, 83.173, DNT, 9.843, DBP, 4.429, DPA, .984, ETOH, .98, H2O,

** PROGRAM BLAKE, VERSION 205.0 **

TE, TEST DAY, 1981 PAGE 19

BLAKE TEST CASE NO. 8: A TYPICAL DOUBLE BASE COMPOSITION

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL T-CAL/M	FORMULA
NC1260	99.986	83.667	-1.6916E+08	C 6000 H 7549 O 9901 N 2431
DNT	.006	9.902	-1.7100E+04	C 7 H 6 O 4 N 2
OBP	.005	4.455	-2.0140E+05	C 16 H 22 O 4
DPA	.001	.990	3.1070E+04	C 12 N 1 H 11
ETOH	.000	.986	-6.6420E+04	C 2 H 6 O 1

THE HEAT OF FORMATION IS -620.94 CAL/GRAM = -1.4154E+08 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C 23.268
H 29.148
O 38.222
N 9.462

***** EXP, V, 5.

THE CONSTANT VOLUME EXPLOSION STATE

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6-12 POTENTIAL AS CORE											
P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHD (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP	
1)	.257607E+04	5.0000	3098.	-309.01	-620.94	2.159	.200	.369	4.438	3.593	1.514

***** PRL,CON,1,PAG,1

***** TIT, BLAKE TEST CASE NO. 9: ISENTROPIC EXPANSION

***** ISOLINE, S, V, 5,7,500

BLAKE TEST CASE NO. 9: ISENTROPIC EXPANSION

ISOLINE

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHD (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP	SIGMA (M/S)	OMEGA (K2/S2)
1) .257607E+04	5.0000	3098.	-304.01	-620.94	2.159	.200	.369	4.438	3.593	1.514	0.000	0.000
2) .101011E+04	9.6535	2625.	-554.37	-790.51	2.159	.104	.352	4.328	3.867	1.378	839.068	1.073
3) .419873E+03	18.6379	2229.	-738.03	-927.54	2.159	.024	.343	4.242	4.001	1.310	1554.801	1.653
4) .179808E+03	35.9842	1897.	-883.78	-1040.47	2.159	.028	.338	4.192	4.068	1.276	2189.330	2.466
5) .782163E+02	69.4746	1617.	-1003.28	-1134.88	2.159	.014	.337	4.184	4.120	1.258	2763.133	2.967
6) .343424E+02	134.1345	1381.	-1103.06	-1214.61	2.159	.007	.347	4.278	4.239	1.245	3287.167	3.384
7) .152486E+02	258.9732	1192.	-1186.92	-1282.55	2.159	.004	.422	4.929	4.863	1.219	3767.508	3.735
8) .693916E+01	500.0000	1061.	-1257.37	-1341.40	2.159	.002	.704	6.884	6.707	1.175	4207.864	4.030

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	1)	2)	3)	4)	5)	6)	7)	8)
CO GAS	1.71772E+01	1.55001E+01	1.65404E+01	1.60730E+01	1.54636E+01	1.46747E+01	1.36468E+01	1.23485E+01
H2O GAS	9.43731E+00	9.16219E+00	8.82675E+00	8.36004E+00	7.79311E+00	6.98071E+00	6.07272E+00	5.23576E+00
CO2 GAS	4.84116E+00	5.12497E+00	5.48685E+00	5.95465E+00	6.56296E+00	7.34366E+00	8.31158E+00	9.37922E+00
N2 GAS	4.48850E+00	4.49427E+00	4.49601E+00	4.49688E+00	4.49692E+00	4.49689E+00	4.49672E+00	4.49676E+00
NH3 GAS	4.35779E+00	4.65203E+00	5.02079E+00	5.49079E+00	6.09590E+00	6.85146E+00	7.63883E+00	8.01445E+00
HCN GAS	9.94077E-03	5.67984E-03	3.89278E-03	3.11378E-03	2.87575E-03	3.03506E-03	3.42786E-03	3.36897E-03
NO GAS	5.21604E-03	1.96078E-03	8.61574E-04	4.20036E-04	2.22097E-04	1.25389E-04	7.27162E-05	3.89533E-05
CH4 GAS	4.59587E-03	6.26081E-04	5.48185E-05	2.90193E-06	8.65779E-08	0.	0.	0.
O2 GAS	3.13556E-04	2.49514E-04	3.17722E-04	6.34445E-04	2.02505E-03	1.03873E-02	7.04118E-02	3.01130E-01
C2H2 GAS	2.41134E-04	1.64792E-05	5.55045E-07	8.66302E-09	0.	0.	0.	0.
C2H4 GAS	9.39751E-06	1.87577E-06	5.25090E-07	1.89607E-07	8.55237E-08	4.71065E-08	2.87000E-08	1.40416E-08
C2N2 GAS	2.95946E-07	9.12222E-08	5.15826E-08	5.03027E-08	8.46805E-08	2.44595E-07	9.71713E-07	2.31363E-06
C GAS	1.36908E-07	1.24617E-08	0.	0.	0.	0.	0.	0.
OH GAS	8.24678E-09	0.	0.	0.	0.	0.	0.	0.
CH3 GAS	3.53322E-02	7.65249E-03	1.09940E-03	1.01911E-04	5.76344E-06	1.91738E-07	4.44158E-09	0.
H GAS	8.59535E-05	2.21906E-05	6.83869E-06	2.37605E-06	9.05027E-07	3.69916E-07	1.53272E-07	5.59183E-08
D GAS	4.74823E-02	4.48791E-03	4.48791E-03	8.57689E-04	1.15390E-04	1.06995E-05	7.68482E-07	7.27744E-08
CHD GAS	2.61484E-04	1.91570E-05	7.00907E-07	1.21715E-08	0.	0.	0.	0.
CH2 GAS	4.76613E-03	9.84641E-04	1.81490E-04	2.81942E-05	3.51496E-06	3.40504E-07	2.74107E-08	2.62572E-09
CN GAS	2.20806E-06	1.66592E-07	1.07731E-08	0.	0.	0.	0.	0.
C(S) SOLID	0.	0.	0.	0.	0.	0.	0.	0.

TOTAL GAS (MOLES/KG) 40.4102 40.3879 40.3817 40.3804 40.3778 40.3410 40.2406 39.7792

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